Supporting Information

Ionic and Neutral Mechanisms for C–H Bond Silylation of Aromatic Heterocycles Catalyzed by Potassium *t*-Butoxide

Shibdas Banerjee,[#,†] Yun-Fang Yang,[#,‡] Ian D. Jenkins,[#,¶] Yong Liang,[‡] Anton A. Toutov,[§] Wen-Bo Liu,[§] David P. Schuman,[§] Robert H. Grubbs,[§] Brian M. Stoltz,[§] Elizabeth H. Krenske,*[,◊] Kendall N. Houk,*[,‡] Richard N. Zare*[,†]

[†]Department of Chemistry, Stanford University, Stanford, CA 94305-5080, USA

[‡]Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095-1569, USA

[¶]Eskitis Institute, Griffith University, Nathan, QLD 4111, Australia

[◊]School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, QLD 4072, Australia

[§]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA

*Emails: e.krenske@uq.edu.au; houk@chem.ucla.edu; zare@stanford.edu

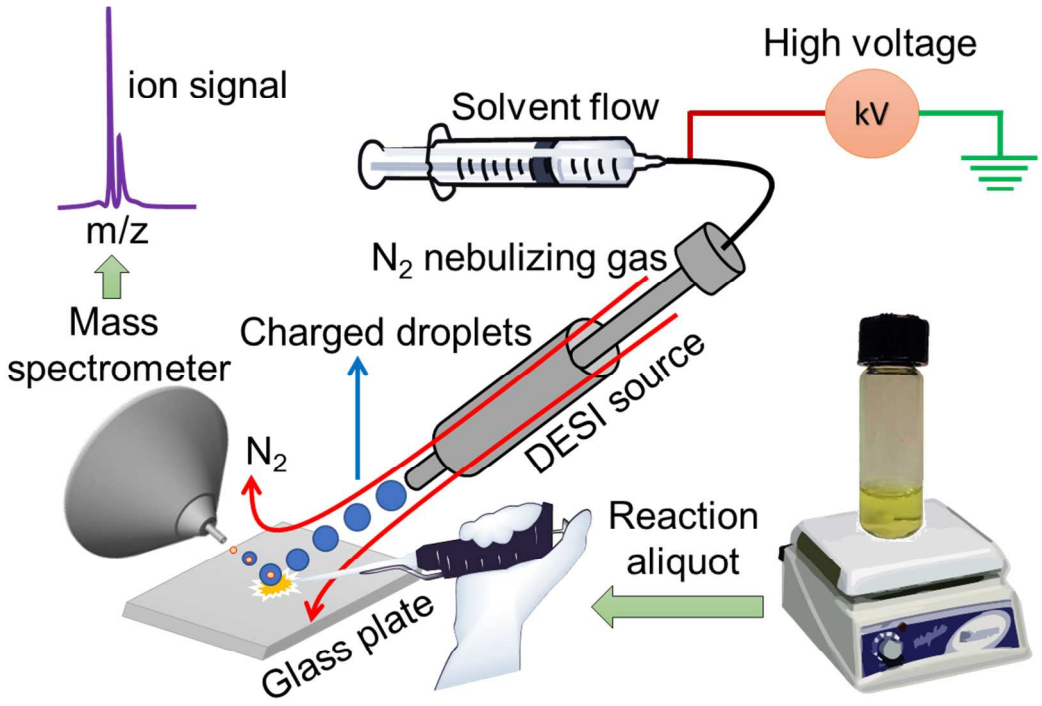


Figure S1. Schematic diagram of DESI-MS set up for intercepting the intermediate(s) and product(s) generated in the reaction mixture. 20 μL reaction aliquot was pipetted out and dispensed immediately on a glass plate under impinging charged microdroplets of polar aprotic solvent (1:1 *v/v* ACN and DMF). Splashing of these microdroplets encapsulated the intermediate and product of the catalytic cycle and transferred them to the mass spectrometer for their subsequent detection. See Experimental Section and Supplementary Note 1 for more details.

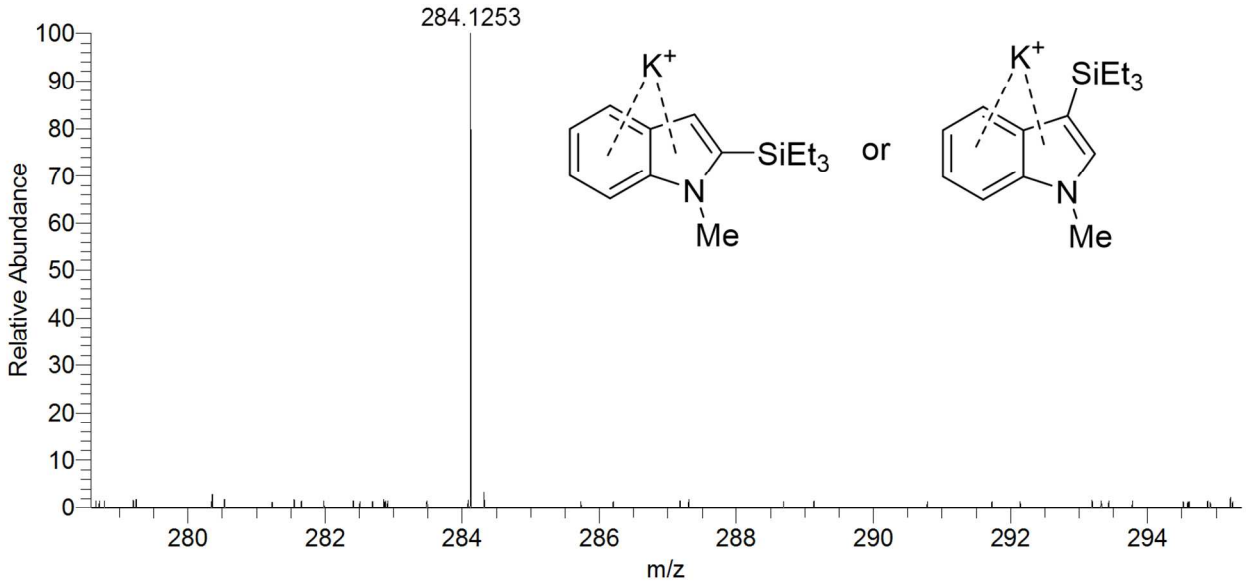


Figure S2. The positive ion mode DESI-MS detected the formation of silylated indole product (potassiated; m/z 284.1252). The experimentally observed m/z value is in good agreement with the theoretically calculated one (m/z 284.1237).

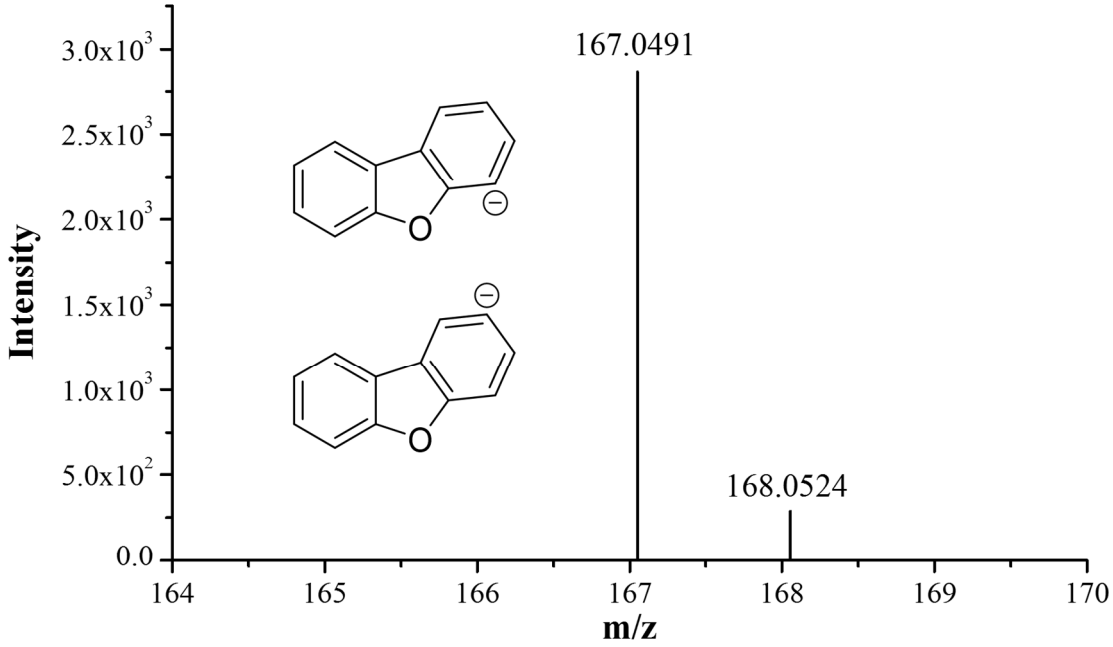


Figure S3. Upper panel shows the scheme of the silylation of dibenzofuran. Lower panel shows the DESI-MS spectrum of the reaction mixture that indicated the presence of deprotonated dibenzofuran species in the reaction mixture.

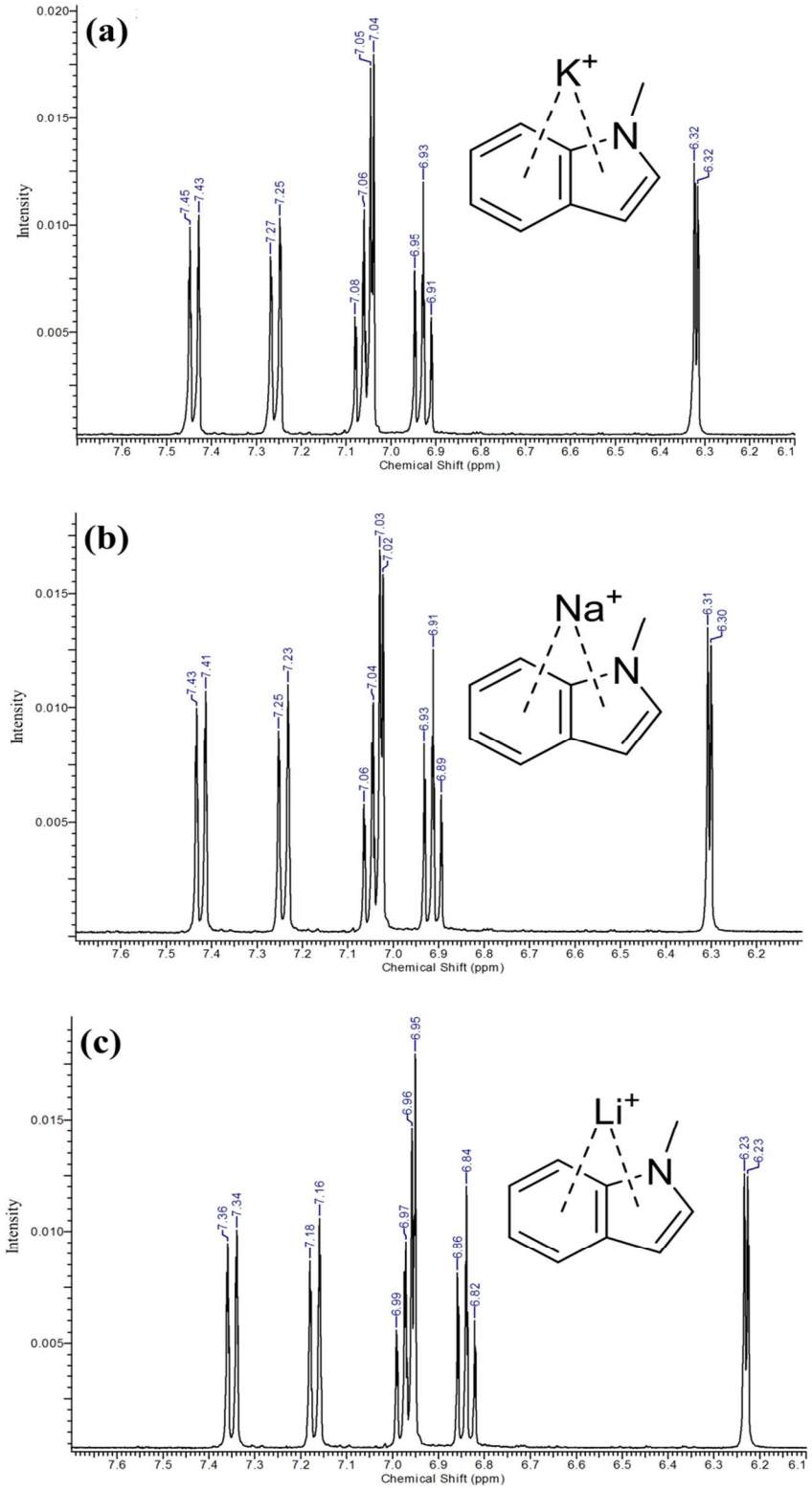


Figure S4. ^{1}H NMR (400 MHz) spectra of 0.03 M 1-methylindole in the methanolic (CD_3OD) solution of (a) 0.3 M potassium acetate, (b) 0.3 M sodium acetate, and (c) 0.3 M lithium acetate. For convenience, the signals from aromatic protons are presented here.

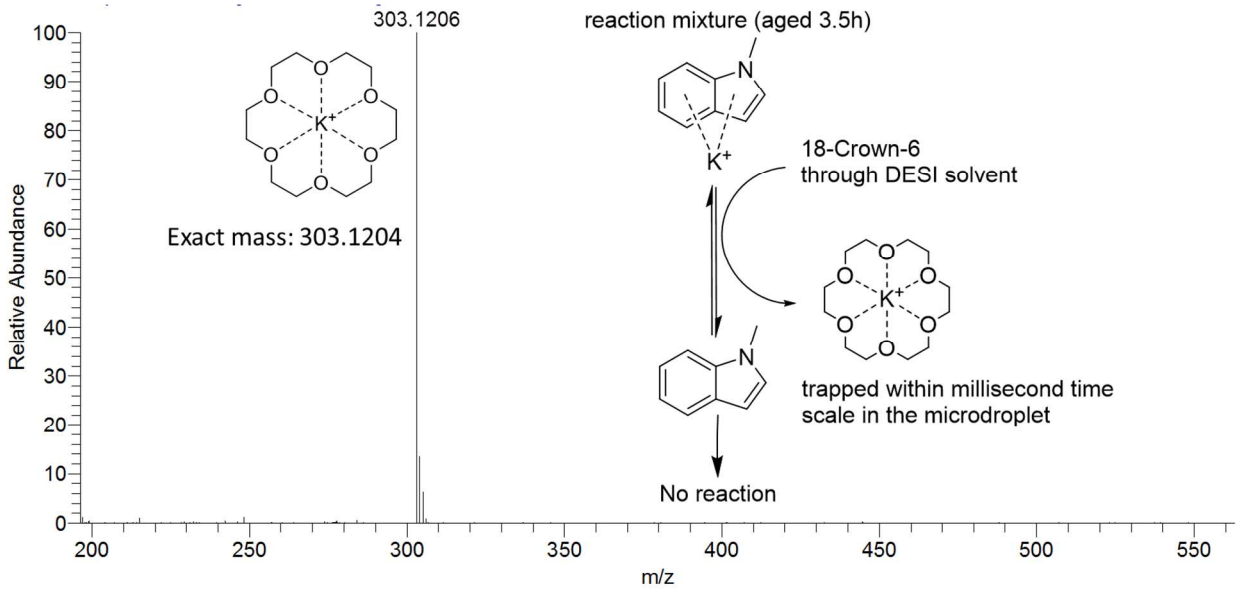


Figure S5. Positive ion mode DESI-mass spectrum showing the formation of potassium-crown ether complex within ms time scale when the reaction mixture (0.1 mmol 1-methylindole + 0.3 mmol triethylsilane + 0.05 mmol KO^{t}Bu in 100 μL dry THF) was bombarded with charged droplets (1:1 ACN/DMF) containing 18-Crown-6. No product or intermediate(s) were detected from this experiment either in positive or in negative ion mode DESI-MS, indicating removal of potassium shuts down the silylation reaction.

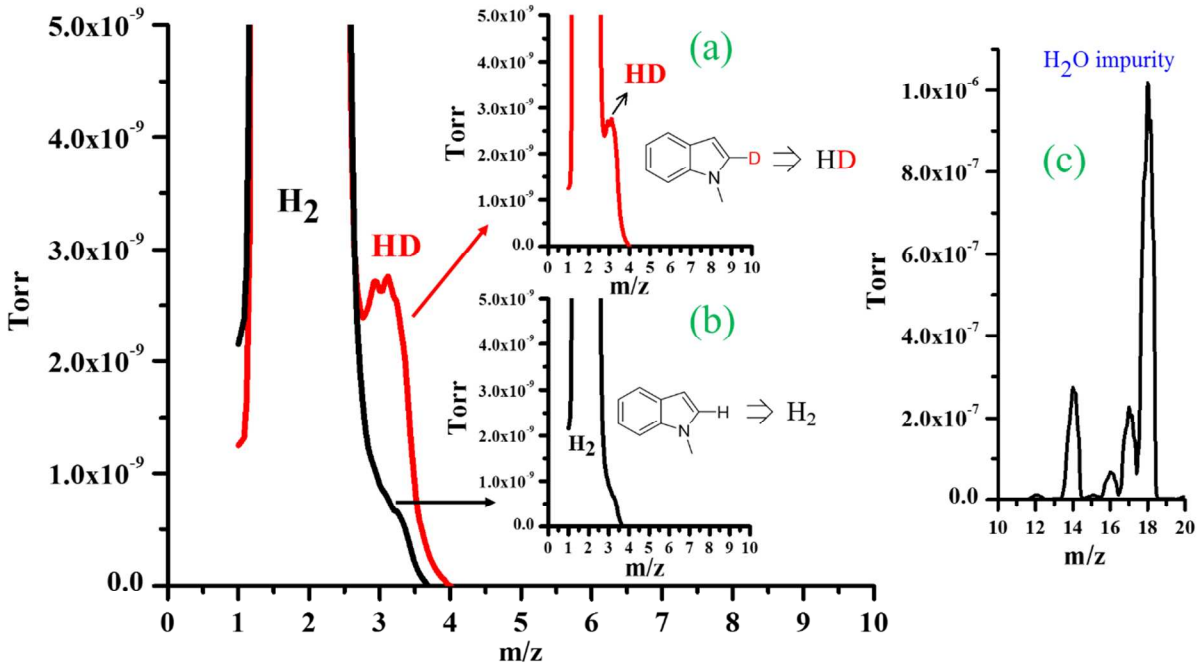


Figure S6. Analyses of the evolving hydrogen gas from the reaction mixture using a residual gas analyzer (RGA; Stanford Research Systems, Sunnyvale, CA): (a) formation of HD from C2-deuterated 1-methylindole substrate, and (b) formation of H_2 from C2-protonated 1-methylindole substrate. Reaction was carried out in 0.02 mmol scale in an airtight 2 dram scintillation vial for 4 days in THF at room temperature in presence of Et_3SiH as silylating agent, and KO^{t}Bu as catalyst. It should be noted that formation of H_2 from the reaction mixtures (a) and (b) might also be contributed by the presence of trace H_2O as impurity in the reaction systems as shown in (c).

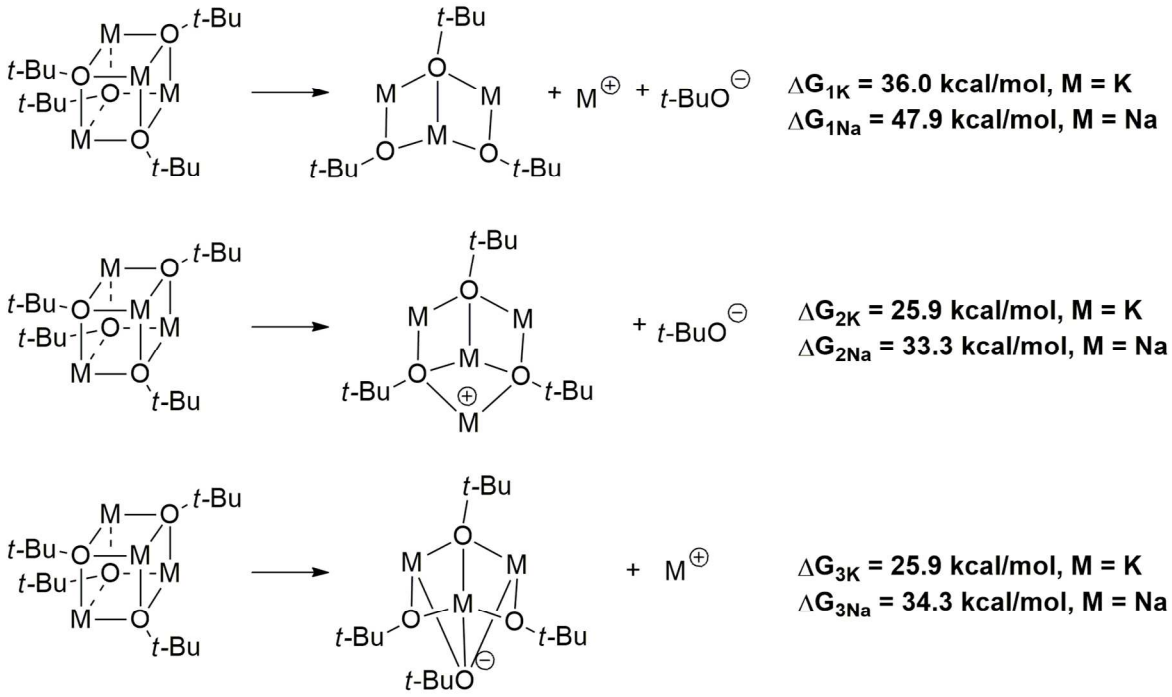


Figure S7. DFT calculation showing the dissociation of $(KO^tBu)_4$ into ions. (Gibbs free energies in THF at 298.15 K were calculated by adding the thermochemical quantities derived from the B3LYP frequencies to the M06-2X solution-phase electronic potential energy.)

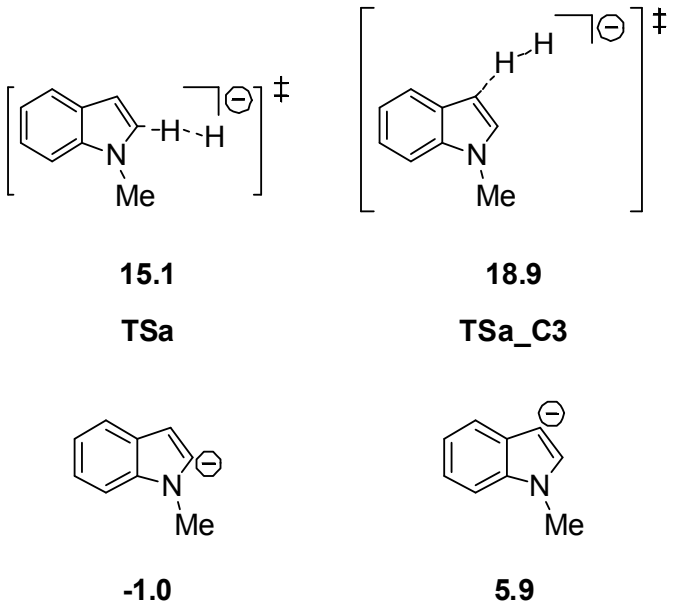


Figure S8. DFT calculation of proton abstractions at C2 and C3 position of N-methylindole.

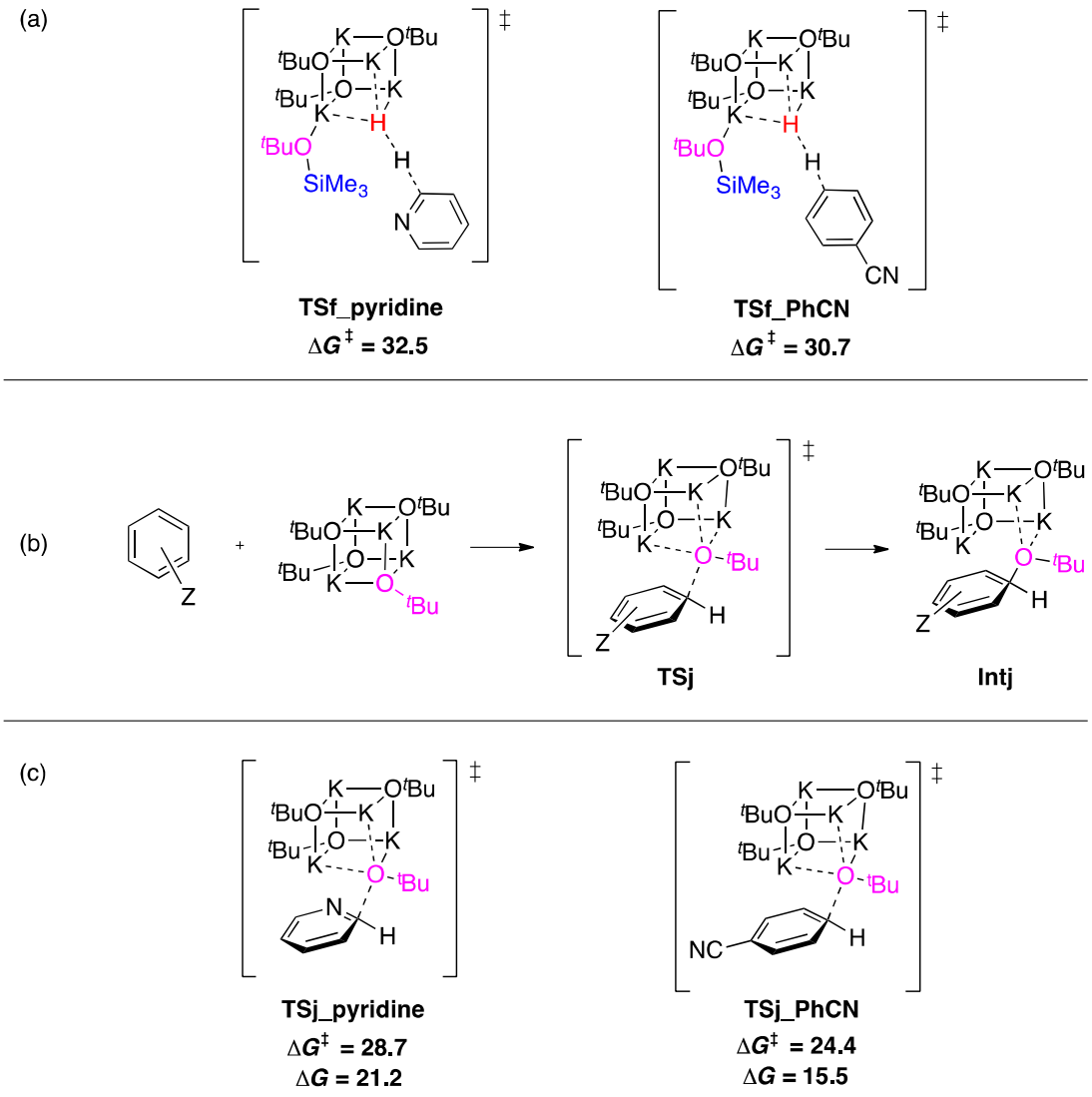


Figure S9. (a) Computed barriers for deprotonation of pyridine and PhCN via transition states analogous to **TSf**. (b) Nucleophilic addition of KO^{t}Bu to electron-deficient (hetero)arenes. (c) Computed barriers for nucleophilic additions of KO^{t}Bu to pyridine and PhCN.$\Delta G^{‡}$ in kcal/mol.

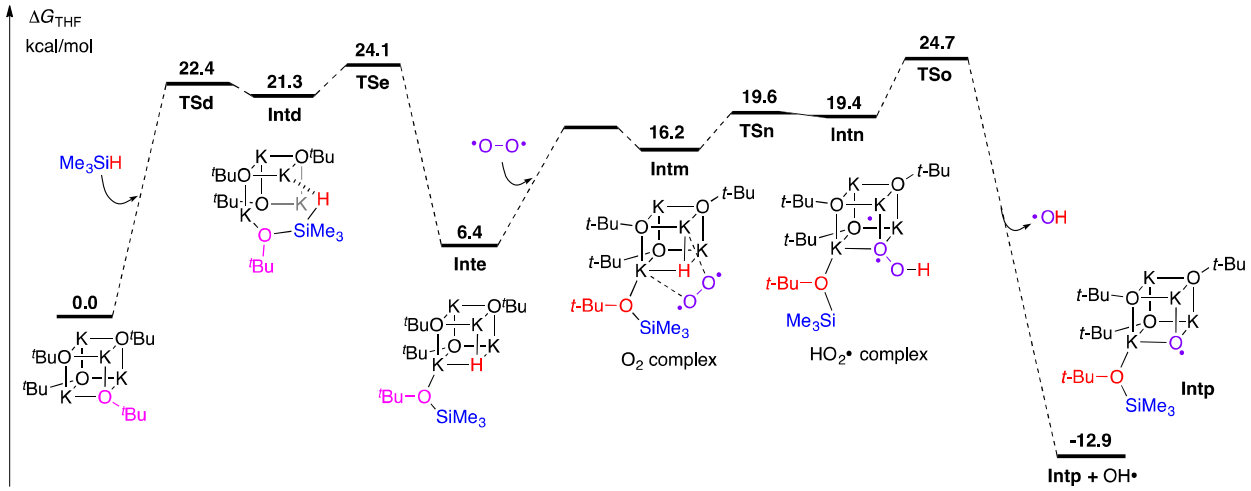


Figure S10. Free energy diagram of a neutral mechanism leading to the formation of radicals in presence of O_2 in the reaction mixture.

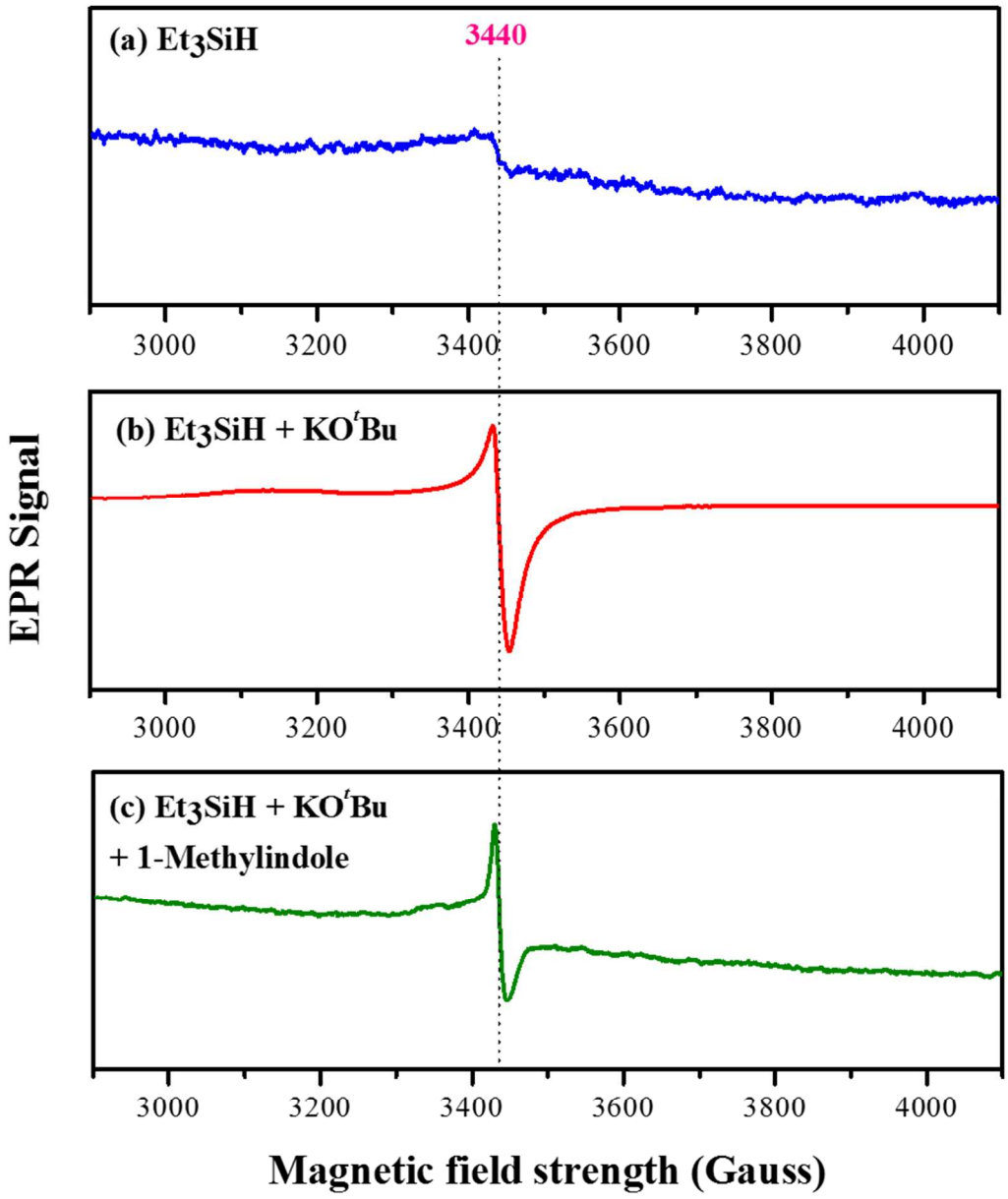


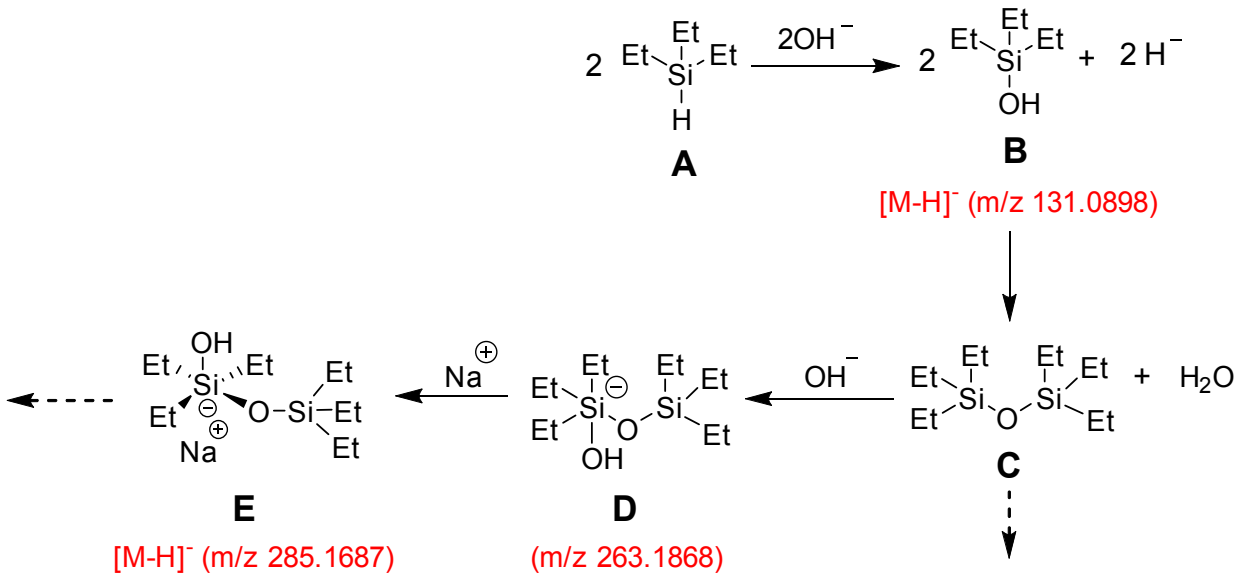
Figure S11. Rapid freeze quench electron spin resonance (EPR) study of (a) triethylsilane (Et_3SiH), (b) mixture of Et_3SiH and KO^tBu in THF, and (c) the reaction mixture in THF.

Supplementary Note 1

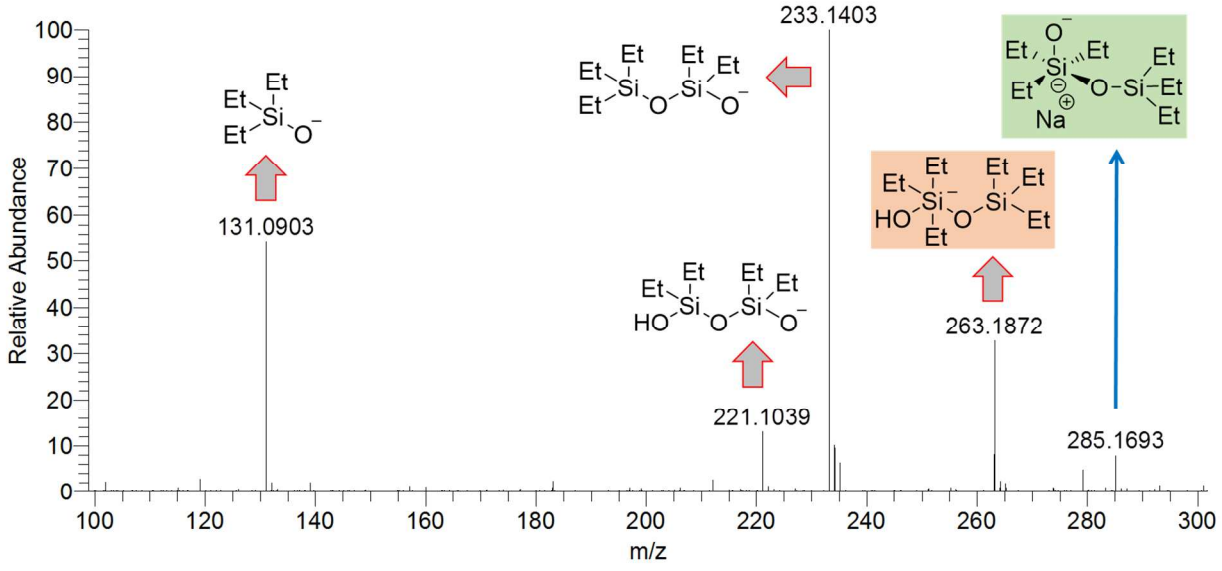
Our earlier studies[1-6] underscored capabilities of the desorption electrospray ionization mass spectrometric (DESI-MS)[7] technique to capture transient intermediates in solution-phase catalytic cycles of complex reactions. To determine the elementary process involved in the KO^{t}Bu catalyzed silylation of heteroaromatic C–H bonds[8] and to understand the reaction on the molecular level, we have employed DESI coupled to a high resolution mass spectrometer to detect intermediates with high mass accuracy. Figure S1 shows the experimental set up of our DESI-MS to monitor the ion signal of the intermediate formed during the progress of the reaction. In this DESI-MS experiment, a spray of charged microdroplets, generated from 1:1 (v/v) acetonitrile (ACN) and dimethylformamide (DMF), was directed toward a sample plate where the reaction mixture was dispensed (see Experimental section for more details). When the incident (primary) microdroplets impact the sample (reaction mixture), they extract species from the sample (reaction mixture) which are found in secondary microdroplets that are formed by the splashing of primary microdroplets.[7] Subsequent solvent evaporation from secondary microdroplets makes the analyte naked in the gas phase and then transfers it to the mass spectrometer for mass-to-charge ratio (m/z) analysis (Figure S1). Typically, the average lifetime of microdroplets in DESI is on the order of milliseconds.[5, 9] Thus, species are generally representatively transferred from solution (reaction mixture) to gas phase rapidly under ambient conditions. In this manner, DESI-MS can provide a 'snapshot' of the reaction in the form of ion signals of the species (reactants, intermediates, and products) associated with the reaction.

Supplementary Note 2

DESI-MS could not detect the pentacoordinate silicon complex **2s** possibly because of the formation of stable neutral ion pair with K^+. However, the DFT calculation has shown (Figure 4) the feasibility of the formation of the pentacoordinate silicon species like **2s** (see Scheme 2). We have confirmed the formation of analogous pentacoordinate silicon species from an experiment where Et_3SiH was treated with NaOH in dimethoxyethane solvent. The reaction proceeds as follows:



Using negative ion mode DESI-MS (Figure S1), we have intercepted the transient pentacoordinate silicon species **D** and its ion pair **E** from the reaction mixture as shown below.



Supplementary Note 3

The transition states analogous to **TSf** for deprotonation of the electron-deficient (hetero)arenes pyridine and PhCN are high in energy, having barriers of $\Delta G^{\ddagger}$ = 32.5 and 30.7 kcal/mol, respectively, compared with 28.3 kcal/mol for 1-methylindole (Figure S9a and Figure 5). Nucleophilic additions of KO^{t}Bu to pyridine and PhCN (Figure S9b,c) have barriers of 28.7 and 24.4 kcal/mol, respectively, and are kinetically favored relative to deprotonation.

DFT-computed energies

Table S1. Energies, enthalpies, and free energies (in Hartree) of the structures calculated with M06-2X/6-311+G(d,p)-CPCM(THF)//B3LYP/6-31G(d).

Structures	ZPE	ΔE	ΔH	ΔG	E	H	G	Imaginary Frequency (cm^{-1})
$tBuO^-$	0.120285	0.126780	0.127724	0.091493	-233.106915	-232.979191	-233.012394	—
K^+	0.000000	0.001416	0.002360	-0.015176	-599.852623	-599.850263	-599.864771	—
KOtBu	0.123876	0.132250	0.133194	0.089516	-833.005741	-832.872547	-832.913197	—
$(KOtBu)_3$	0.373819	0.402210	0.403154	0.308232	-2499.076483	-2498.673329	-2498.76522	—
$(KOtBu)_4$	0.498948	0.537092	0.538036	0.423883	-3332.132729	-3331.594693	-3331.70582	—
Na^+	0.000000	0.001416	0.00236	-0.014429	-162.189925	-162.187565	-162.201326	—
NaOtBu	0.124504	0.132747	0.133691	0.091144	-395.346359	-395.212668	-395.252187	—
$(NaOtBu)_3$	0.376694	0.404037	0.404981	0.314435	-1186.114703	-1185.709722	-1185.797240	—
$(NaOtBu)_4$	0.503381	0.539676	0.540621	0.432343	-1581.528698	-1580.988077	-1581.093327	—
$K_4(OtBu)_3^+$	0.376381	0.405929	0.406873	0.313063	-3098.965258	-3098.558385	-3098.649167	—
$Na_4(OtBu)_3^+$	0.378955	0.407455	0.408399	0.317739	-1348.343957	-1347.935558	-1348.023190	—
$K_3(OtBu)_4^-$	0.496076	0.532777	0.533721	0.419731	-2732.219468	-2731.685747	-2731.796709	—
$Na_3(OtBu)_4^-$	0.499759	0.535003	0.535947	0.42765	-1419.26656	-1418.730613	-1418.835882	—
$HSiMe_3$	0.119775	0.127259	0.128203	0.089443	-409.808109	-409.679906	-409.715638	—
N-Me-Indole	0.157986	0.166006	0.166950	0.124908	-403.061521	-402.894571	-402.933585	—
Hydride	0.000000	0.001416	0.002360	-0.010000	-0.624003	-0.621643	-0.630975	—
H_2	0.010145	0.012505	0.013450	-0.001342	-1.168439	-1.154989	-1.166753	—
$tBuOSiMe_3$	0.239087	0.253167	0.254111	0.199885	-642.300631	-642.046520	-642.097718	—
Inta	0.243120	0.257862	0.258806	0.203152	-642.926999	-642.668193	-642.720819	—
TSa	0.155160	0.163891	0.164835	0.121793	-403.664673	-403.499838	-403.539852	-1069.5
TSa_C3	0.153846	0.163207	0.164151	0.119213	-403.655944	-403.491793	-403.533703	-1082.0
N-Me-Indole_anion	0.142817	0.150653	0.151597	0.110479	-402.512185	-402.360588	-402.398678	—
N-Me-Indole_anion_C3	0.142179	0.150330	0.151274	0.108679	-402.499445	-402.348171	-402.387738	—
Intb	0.383311	0.407081	0.408025	0.327581	-1044.814310	-1044.406285	-1044.483701	—

TSb	0.383239	0.406260	0.407204	0.330353	-1044.809572	-1044.402368	-1044.476191	-58.5
Intc	0.384344	0.407453	0.408397	0.332947	-1044.819947	-1044.411550	-1044.483972	—
TSc	0.382512	0.405746	0.406690	0.328919	-1044.806966	-1044.400276	-1044.475019	-82.8
N-Me-Indole_pro	0.260259	0.276207	0.277151	0.217055	-811.697822	-811.420671	-811.477739	—
N-Me-Indole_pro_C3	0.260073	0.276139	0.277083	0.216367	-811.700813	-811.42373	-811.481418	—
TSd	0.622044	0.667165	0.668109	0.541711	-3741.924723	-3741.256614	-3741.379994	-90.2
Intd	0.622313	0.667948	0.668892	0.541955	-3741.926735	-3741.257843	-3741.381762	—
TSe	0.618655	0.664534	0.665478	0.535718	-3741.915924	-3741.250446	-3741.377187	-231.4
Inte	0.619131	0.665861	0.666805	0.531810	-3741.940262	-3741.273457	-3741.405434	—
TSf	0.773989	0.830614	0.831558	0.675041	-4144.982118	-4144.150560	-4144.304058	-570.4
TSf_C3	0.774142	0.830830	0.831774	0.674920	-4144.973929	-4144.142155	-4144.295990	-482.7
Intf	0.761241	0.816695	0.817639	0.664776	-4143.833776	-4143.016137	-4143.165982	—
TSg	0.762252	0.815868	0.816812	0.671659	-4143.817092	-4143.000280	-4143.142414	-10.9
Intg	0.762373	0.816757	0.817702	0.670197	-4143.819724	-4143.002023	-4143.146508	—
TSh	0.762154	0.816827	0.817771	0.668159	-4143.814177	-4142.996406	-4143.142999	—
Inth	0.762256	0.816853	0.817797	0.669162	-4143.818656	-4143.000859	-4143.146475	—
TSi	0.761384	0.815531	0.816475	0.668928	-4143.810704	-4142.994228	-4143.138757	-54.0
$K_4(OtBu)_3(tBuOSiMe_3)^+$	0.616106	0.661838	0.662782	0.530981	-3741.275719	-3740.612937	-3740.741719	—
$K_4(OtBu)_3^+$	0.376096	0.405751	0.406696	0.312248	-3098.965329	-3098.558633	-3098.650063	—
(2-indolyl)$SiMe_3(OtBu)^-$	0.384338	0.407451	0.408395	0.332923	-1044.819975	-1044.411581	-1044.484034	—
$(NaOtBu)_4$	0.504205	0.540033	0.540977	0.439206	-1581.526065	-1580.985089	-1581.083841	—
TSf_Na	0.777161	0.832214	0.833158	0.682147	-2394.356023	-2393.522865	-2393.670857	-804.4
Thiophene	0.066884	0.070960	0.071904	0.039644	-552.971213	-552.899310	-552.928551	—
TSf_thiophene	0.683159	0.735708	0.736653	0.589614	-4294.896013	-4294.159360	-4294.303380	-684.5
Furan	0.070203	0.073918	0.074863	0.043931	-229.992451	-229.917588	-229.945501	—
TSf_furan	0.686316	0.738423	0.739367	0.593386	-3971.912028	-3971.172660	-3971.315623	-625.1
N-Me-pyrrole	0.110674	0.116254	0.117198	0.081658	-249.437434	-249.320236	-249.352758	—
TSf_N-Me-pyrrole	0.727268	0.781138	0.782083	0.633021	-3991.352778	-3990.570695	-3990.716738	-529.1
Pyridine	0.089033	0.093302	0.094246	0.062287	-248.242810	-248.148564	-248.177504	—
TSf_pyridine	0.704562	0.757489	0.758433	0.609894	-3990.154306	-3989.395873	-3989.541393	-521.9
PhCN	0.099441	0.105546	0.106490	0.069814	-324.444163	-324.337674	-324.371331	—
TSf_PhCN	0.715502	0.770287	0.771232	0.617926	-4066.358930	-4065.587698	-4065.737984	-456.1
TSj_pyridine	0.590472	0.632997	0.633942	0.512035	-3580.346766	-3579.712824	-3579.831713	-187.7
Intj_pyridine	0.590824	0.633870	0.634815	0.510001	-3580.356754	-3579.721939	-3579.843734	—
TSj_PhCN	0.599303	0.644431	0.645375	0.515520	-3656.551030	-3655.905655	-3656.032491	-57.9
Intj_PhCN	0.601787	0.646729	0.647673	0.518858	-3656.568512	-3655.920839	-3656.046636	—
TSk	0.881394	0.941543	0.942487	0.780165	-4225.568199	-4224.625712	-4224.785015	-684.9
Intk	0.615028	0.661124	0.662069	0.528782	-3741.325639	-3740.663570	-3740.793838	—
7	0.878646	0.938063	0.939007	0.781308	-4225.066563	-4224.127556	-4224.282237	—
TEMPO	0.263321	0.275359	0.276304	0.226574	-483.635317	-483.359013	-483.405724	—
TEMPO-H	0.275299	0.287401	0.288345	0.239675	-484.249720	-483.961375	-484.007026	—
O_2	0.003778	0.006141	0.007085	-0.016201	-150.307691	-150.300606	-150.320873	—
Intm	0.623966	0.674067	0.675011	0.532896	-3892.246600	-3891.571589	-3891.710685	—

TSn	0.622740	0.672757	0.673701	0.531391	-3892.239643	-3891.565941	-3891.705232	-649.3
Intn	0.626104	0.676651	0.677595	0.532818	-3892.241506	-3891.563910	-3891.705669	—
TSo	0.623282	0.673649	0.674593	0.530141	-3892.230317	-3891.555724	-3891.697157	-1050.2
OH radical	0.008304	0.010665	0.011609	-0.008638	-75.731055	-75.719446	-75.736675	—
Intp	0.616712	0.664280	0.665225	0.529551	-3816.552969	-3815.887745	-3816.020399	—

Cartesian coordinates of the structures:

$tBuO^-$

C	0.76930400	-1.24460500	-0.43646700
C	-0.00013200	0.00003900	0.15967000
H	1.80070000	-1.23142400	-0.05612200
H	0.29528800	-2.16143000	-0.05785000
H	0.80692800	-1.30343600	-1.54066300
C	-1.46235500	-0.04349000	-0.43746700
C	0.69389900	1.28820400	-0.43640400
H	-2.01975600	0.82455800	-0.05747100
H	-1.53139800	-0.04446200	-1.54167000
H	-1.96691400	-0.94406300	-0.05922000
H	0.72813100	1.34844400	-1.54055500
H	0.16624100	2.17542300	-0.05815900
H	1.72413700	1.33653400	-0.05572100
O	-0.00095700	-0.00012900	1.48392900

KOtBu

C	1.61010700	1.01764800	-1.04001700
C	1.07202700	0.00006500	-0.00009800
H	1.23720600	0.75376100	-2.03823200
H	1.23781900	2.02141000	-0.79701900
H	2.70796700	1.05905000	-1.08255000
C	1.61109200	0.39186400	1.40093900
C	1.60994700	-1.40984100	-0.36130400
H	1.23813600	-0.31922100	2.14954100
H	2.70904000	0.40639600	1.45700600
H	1.23997100	1.38906000	1.67139700
H	2.70776000	-1.46832900	-0.37355000
H	1.23451300	-2.14187700	0.36546100
H	1.23915100	-1.70074000	-1.35273600
O	-0.30080900	0.00007000	0.00000900
K	-2.55600700	0.00008000	0.00018400

$(KOtBu)_3$

O	0.00015600	1.99898400	-0.24404000
O	2.30339200	-0.91026700	-0.11571700
O	-2.30411900	-0.90944400	-0.11548200
K	-2.26639700	1.24327100	-1.24738100
K	2.26606000	1.24224500	-1.24814300
K	-0.00020800	-0.56204900	0.94732200

C	0.00059000	3.14890900	0.53473600
C	3.16018400	-1.98185400	0.04070200
C	-3.16059500	-1.98133200	0.04061100
C	-1.25165200	4.02460900	0.24927900
H	-2.16932900	3.48261300	0.52301200
H	-1.25793200	4.96449300	0.81609000
H	-1.29717900	4.27731700	-0.81940200
C	1.25368300	4.02348900	0.24957000
H	1.26073900	4.96329100	0.81650600
H	2.17081200	3.48060700	0.52337600
H	1.29960200	4.27631400	-0.81906900
C	0.00027300	2.79074600	2.04497300
H	0.89026300	2.19420700	2.28829200
H	0.00058600	3.67297100	2.69869900
H	-0.89027300	2.19496300	2.28810400
C	-4.63064600	-1.49411200	0.15035400
H	-4.91351900	-0.95694000	-0.76707100
H	-5.35112900	-2.31138700	0.29272500
H	-4.72764300	-0.79908600	0.99443600
C	-3.04955500	-2.94819200	-1.16615400
H	-2.01491100	-3.30061700	-1.26250500
H	-3.70717800	-3.82429700	-1.08088200
H	-3.30798200	-2.41724400	-2.09267400
C	-2.82034400	-2.77429200	1.33264900
H	-1.79361600	-3.16344500	1.27430400
H	-2.88873800	-2.10955600	2.20464100
H	-3.48765000	-3.62977200	1.50422400
C	3.04905500	-2.94938900	-1.16551200
H	3.70702300	-3.82521100	-1.08001000
H	2.01450200	-3.30223300	-1.26130200
H	3.30695200	-2.41884200	-2.09240900
C	4.63014600	-1.49420200	0.14976400
H	4.72717900	-0.79863700	0.99340000
H	5.35087800	-2.31120000	0.29245800
H	4.91266400	-0.95753000	-0.76806700
C	2.82050900	-2.77419000	1.33327200
H	2.88885700	-2.10893200	2.20486900
H	1.79390000	-3.16371700	1.27536900
H	3.48814700	-3.62934300	1.50519000

$(KOtBu)_4$

O	-1.35223000	-1.22398900	-1.39308300
O	1.33776900	-1.41923500	1.20966400
O	-1.29895000	1.23549700	1.43282500
O	1.31340800	1.40712700	-1.24975800
K	1.27675600	-1.21412600	-1.41362300
K	-1.29083300	-1.38866300	1.22775500
K	-1.31490700	1.39972200	-1.18877700
K	1.32898100	1.20247200	1.37432100
C	-2.17096600	-1.94544200	-2.24970100
C	2.14883000	-2.29018100	1.92258000
C	-2.08721500	1.96281600	2.31274900
C	2.10935200	2.27300200	-1.98552700
C	-1.89258000	-1.56766700	-3.72898400
H	-0.84297100	-1.77204500	-3.98192500
H	-2.52292000	-2.11815700	-4.44009400
H	-2.06704600	-0.49417300	-3.88575100
C	-3.66747600	-1.66064500	-1.95382900
H	-4.35011800	-2.21715100	-2.60988100
H	-3.90587600	-1.92758500	-0.91510700
H	-3.88178300	-0.58988600	-2.07707600
C	-1.92997000	-3.47011900	-2.08922200
H	-0.88052600	-3.71272900	-2.30610600

H	-2.13329200	-3.77922000	-1.05460000
H	-2.55996000	-4.07853500	-2.75185300
C	1.83813600	-3.76443600	1.55039700
H	1.99675500	-3.92581800	0.47513500
H	2.46150200	-4.48660800	2.09439300
H	0.78646900	-3.99726900	1.76767500
C	1.92916900	-2.12320100	3.44978300
H	2.55359700	-2.79699300	4.05164200
H	2.15595900	-1.09227600	3.75493600
H	0.87873600	-2.31959800	3.70516600
C	3.64714000	-2.02295400	1.61951400
H	3.90825500	-0.98855300	1.88195200
H	4.32386700	-2.69102000	2.16890000
H	3.84633300	-2.15169300	0.54648000
C	1.83962800	2.11308400	-3.50544100
H	0.78355000	2.32039100	-3.72671300
H	2.45104900	2.78284100	-4.12490100
H	2.04657300	1.08102000	-3.82059900
C	1.82430000	3.74880800	-1.59920300
H	2.01885500	3.90533800	-0.52912000
H	2.43652100	4.46703100	-2.16079400
H	0.76838600	3.99187500	-1.78187900
C	3.61401200	1.99110000	-1.73114300
H	3.84836800	2.11430600	-0.66458900
H	3.85711100	0.95527600	-2.00502600
H	4.27906900	2.65484500	-2.29968500
C	-1.83877100	3.48563800	2.14612900
H	-2.44463500	4.09861700	2.82681300
H	-0.78163800	3.71971100	2.33291200
H	-2.06920200	3.79703800	1.11789400
C	-3.59377600	1.69013700	2.05955700
H	-3.81305500	0.62103900	2.18837700
H	-4.25291300	2.25161800	2.73510900
H	-3.85963200	1.95971200	1.02820200
C	-1.76980400	1.58183100	3.78332400
H	-1.94855300	0.50970400	3.94460500
H	-0.71175700	1.77741800	4.00622400
H	-2.37504500	2.13699300	4.51238200

$HSiMe_3$

C	1.65126200	-0.70689500	0.22213800
H	1.70175600	-0.72850500	1.31767000
H	1.79912900	-1.73223900	-0.13686300
H	2.49496800	-0.10560400	-0.13664300
C	-0.21332700	1.78329500	0.22197400
H	0.60027100	2.42409300	-0.13790700
H	-1.15625700	2.21310500	-0.13607500
H	-0.21878500	1.83812100	1.31758600
C	-1.43812000	-1.07619200	0.22208500
H	-2.39990700	-0.68986500	-0.13542000
H	-1.34100400	-2.10714800	-0.13817300
H	-1.48100900	-1.11032300	1.31764100
Si	0.00013800	-0.00018300	-0.37553700
H	0.00001200	-0.00031900	-1.87147700

NaOtBu

C	1.14721600	1.45528400	-0.01297000
C	0.61947700	-0.00001700	-0.00006800
H	0.77577000	1.97449500	-0.90533400
H	0.77319000	1.99106000	0.86845300
H	2.24439000	1.51313900	-0.01193300
C	1.14518000	-0.71563600	1.26792800
C	1.14957800	-0.73951700	-1.25250600

H	0.77266300	-1.74741100	1.28993500
H	2.24227800	-0.74372100	1.32061800
H	0.77029800	-0.20292800	2.16258500
H	2.24687000	-0.76732400	-1.30104300
H	0.77827400	-1.77197300	-1.25577900
H	0.77708800	-0.24467100	-2.15813500
O	-0.75940500	-0.00017100	-0.00229800
Na	-2.69766200	0.00000100	-0.00048000

$(NaOtBu)_3$

O	0.02156900	1.86375700	-0.39069100
O	2.05954600	-0.76137900	-0.03349500
O	-2.09149100	-0.71144400	-0.08200900
C	0.03590500	3.11875700	0.23915600
C	2.97151500	-1.80996700	0.04157400
C	-3.01974500	-1.74054600	0.04611900
C	-1.04531000	4.04107400	-0.37573100
H	-2.05156300	3.63181000	-0.19217500
H	-1.03737000	5.05202200	0.05015200
H	-0.89563300	4.12639500	-1.45988000
C	1.41471500	3.80110000	0.05158500
H	1.46289400	4.79884600	0.50409400
H	2.20606600	3.20065700	0.52598000
H	1.64065600	3.91346400	-1.01910500
C	-0.23659300	2.96186000	1.75184000
H	0.53415300	2.32851400	2.20936100
H	-0.24355800	3.92266400	2.28217300
H	-1.20873600	2.47811200	1.91185400
C	-4.45745700	-1.17432300	-0.04443800
H	-4.60420900	-0.68302300	-1.01764000
H	-5.23041600	-1.94725300	0.05793500
H	-4.61354700	-0.42661500	0.74372800
C	-2.81748400	-2.78204500	-1.07824200
H	-1.80155200	-3.19279800	-1.02906100
H	-3.52943000	-3.61591300	-1.01795600
H	-2.93584700	-2.30130500	-2.05818900
C	-2.85094100	-2.43918700	1.41680700
H	-1.84353300	-2.87034500	1.49584100
H	-2.97326400	-1.70674600	2.22462900
H	-3.57493000	-3.24949400	1.57350700
C	2.42951400	-3.04220500	-0.71887700
H	3.12049200	-3.89532100	-0.69424700
H	1.47584000	-3.36334300	-0.28078800
H	2.24278600	-2.77983300	-1.76773400
C	4.32071700	-1.38890000	-0.59162100
H	4.72336500	-0.51347700	-0.06350700
H	5.07883500	-2.18210700	-0.55626600
H	4.16883900	-1.11918900	-1.64689800
C	3.21852100	-2.19140400	1.52010600
H	3.58933600	-1.31926100	2.07249200
H	2.27662000	-2.51010100	1.98603300
H	3.94468700	-3.00726000	1.63312100
Na	-1.94968600	1.14968300	-1.02837200
Na	-0.01849800	-0.45107900	0.53813600
Na	2.00290100	1.11759100	-0.96136000

$(NaOtBu)_4$

O	1.11330300	-1.15663000	-1.26273000
O	-1.73097700	-0.98967600	0.47161100
O	-0.46237700	1.76602200	-0.91121300
O	1.05880200	0.36050300	1.70742100
C	1.87642300	-1.94427100	-2.12795000
C	-2.90698700	-1.65775500	0.82109000

C	-0.78216600	2.97013400	-1.54306300
C	1.81569300	0.63437400	2.84914300
C	2.14289800	-3.32995400	-1.49377000
H	1.18966800	-3.83418700	-1.28443500
H	2.73773900	-3.98893600	-2.13939800
H	2.68696400	-3.20967700	-0.54656000
C	3.23398100	-1.25930300	-2.41484200
H	3.87453700	-1.84283800	-3.08843500
H	3.06722300	-0.27723400	-2.87909800
H	3.78232900	-1.10926700	-1.47477800
C	1.12718600	-2.14510900	-3.46656200
H	0.16755800	-2.64936500	-3.28615100
H	0.92445300	-1.17011600	-3.93046900
H	1.69234100	-2.74953200	-4.18775400
C	-2.57226800	-3.02471200	1.46395800
H	-1.96364200	-2.87389400	2.36647000
H	-3.46561500	-3.59280200	1.75381300
H	-1.99796600	-3.63922200	0.75718100
C	-3.77782400	-1.89724500	-0.43493400
H	-4.71732200	-2.41897100	-0.21156700
H	-4.02977200	-0.93598500	-0.90338200
H	-3.22284400	-2.50282200	-1.16477100
C	-3.71740600	-0.81611300	1.83550500
H	-3.97596400	0.15594000	1.39292300
H	-4.65179000	-1.30160300	2.14531500
H	-3.11620000	-0.63801600	2.73771600
C	3.08752700	1.42943900	2.46759400
H	2.80627200	2.37405000	1.98185400
H	3.71672100	1.67233000	3.33340600
H	3.69701700	0.84474200	1.76440100
C	0.98680700	1.47307800	3.85050400
H	0.08068000	0.92285000	4.13848400
H	1.53980900	1.71435600	4.76737700
H	0.68297800	2.41990800	3.38282600
C	2.24193600	-0.68466100	3.53605600
H	1.35188000	-1.26017600	3.82549200
H	2.83610900	-1.29299700	2.84036500
H	2.84465100	-0.52181800	4.43879600
C	0.50507800	3.77713600	-1.83560600
H	0.30563200	4.73944300	-2.32429300
H	1.03930300	3.98025200	-0.89738200
H	1.16825400	3.19835700	-2.49355700
C	-1.51156000	2.69479000	-2.87943200
H	-2.43733600	2.13325700	-2.69153700
H	-1.78063200	3.61319300	-3.41691900
H	-0.86942800	2.09474300	-3.53858100
C	-1.70679600	3.81845900	-0.63775400
H	-2.62885100	3.26213700	-0.42029500
H	-1.20161800	4.03705700	0.31335100
H	-1.99107600	4.77570700	-1.09321100
Na	0.40921400	-1.60661800	0.82665400
Na	-1.01458200	1.03498300	1.14947700
Na	1.55338600	0.89104100	-0.42966100
Na	-0.96867300	-0.33761800	-1.54170100

$K_4(OtBu)_3^+$

O	-2.05152800	0.56526500	-0.19895100
O	1.51454100	1.49410000	-0.19894200
O	0.53669300	-2.05813000	-0.19801700
K	-1.82520200	-1.80029200	-1.23403600
K	-0.64722200	2.48261500	-1.23409100
K	2.47284100	-0.68102100	-1.23475200
K	0.00029000	0.00121300	1.42548400

C	-3.31040500	0.91013200	0.30659200
C	2.44425000	2.41022200	0.30675100
C	0.86576500	-3.32152100	0.30684000
C	-4.39741000	-0.08984500	-0.16636300
H	-4.18716900	-1.10004600	0.21701700
H	-5.40182700	0.17494400	0.18385800
H	-4.43099000	-0.12499800	-1.26464500
C	-3.73623100	2.32447200	-0.16650100
H	-4.73537900	2.60822800	0.18399700
H	-3.04051700	3.08677800	0.21623900
H	-3.74774700	2.37154900	-1.26480600
C	-3.29404000	0.90622200	1.85616000
H	-2.55416100	1.62864600	2.22994500
H	-4.26213800	1.17232100	2.29733900
H	-3.02681300	-0.09229700	2.23107100
C	-0.14829300	-4.39541400	-0.16606000
H	-0.18395000	-4.42864300	-1.26433600
H	0.10345600	-5.40314200	0.18409600
H	-1.15551900	-4.17165800	0.21738600
C	2.27452300	-3.76457100	-0.16704700
H	3.04530300	-3.07849900	0.21610700
H	2.54665500	-4.76745600	0.18207600
H	2.32111700	-3.77565400	-1.26539800
C	0.86247200	-3.30582300	1.85637900
H	1.59513800	-2.57621500	2.23037700
H	-0.13210800	-3.02462500	2.23161900
H	1.11507900	-4.27788400	2.29679500
C	3.88274000	2.06246100	-0.15696700
H	4.63037700	2.78308100	0.19437100
H	4.18763700	1.07875100	0.23152200
H	3.93522500	2.04440100	-1.25499900
C	2.13076200	3.85055600	-0.17514900
H	1.15038900	4.17986600	0.20172900
H	2.86379700	4.58650600	0.17506500
H	2.12254400	3.89172600	-1.27366500
C	2.42445500	2.40636000	1.85635800
H	1.42484900	2.67896500	2.22453600
H	2.67552000	1.40594700	2.23735800
H	3.13863200	3.11223400	2.29715900

$Na_4(OtBu)_3^+$

O	-0.96430000	1.63741800	-0.17323400
O	1.89909200	0.01860300	-0.16952400
O	-0.93377400	-1.65042100	-0.16630500
C	-1.66395400	2.82616800	0.14417200
C	3.27995400	0.03247600	0.14175400
C	-1.61625200	-2.85216600	0.13992700
C	-3.09500600	2.76466800	-0.43553000
H	-3.65981400	1.93639700	0.02086400
H	-3.67217600	3.67626800	-0.24501200
H	-3.06130500	2.62148000	-1.52541700
C	-0.93418500	4.04491900	-0.46341400
H	-1.45198400	4.99087000	-0.26987400
H	0.07310700	4.14608900	-0.02945900
H	-0.84791200	3.93645900	-1.55429300
C	-1.74372200	2.99302700	1.67503900
H	-0.73420100	3.04558300	2.10395000
H	-2.28024700	3.90107500	1.97320600
H	-2.26390300	2.13576200	2.12281000
C	-3.02617100	-2.83443800	-0.49248600
H	-2.95662500	-2.70116800	-1.58173500
H	-3.58529500	-3.75912900	-0.31180900
H	-3.62997700	-2.01753800	-0.06609700

C	-0.83485400	-4.05905800	-0.42651600
H	0.15866600	-4.12903800	0.04386200
H	-1.33482700	-5.01585400	-0.24005500
H	-0.71324700	-3.96146300	-1.51528900
C	-1.74759900	-3.00515300	1.66848200
H	-0.75349400	-3.03020700	2.13434100
H	-2.30257100	-2.15541100	2.08777500
H	-2.27379500	-3.92233300	1.95697800
C	3.94761000	-1.26288300	-0.37265200
H	5.02511300	-1.29387700	-0.17717400
H	3.51334800	-2.14314100	0.12686000
H	3.81171400	-1.35968100	-1.46001800
C	3.96054100	1.24303700	-0.53519900
H	3.54664500	2.18645200	-0.14497100
H	5.04044000	1.28021600	-0.35370600
H	3.81117900	1.20777600	-1.62378200
C	3.47185700	0.12928200	1.66845300
H	3.00318800	1.04517600	2.05218600
H	3.00379900	-0.73110700	2.16509500
H	4.52818600	0.14775700	1.96024400
Na	0.00177700	0.00425800	1.07056500
Na	-2.19692000	-0.02019800	-0.95916400
Na	1.07430000	1.89962000	-0.97940100
Na	1.12161700	-1.90199700	-0.93646800

$K_3(OtBu)_4^-$

O	-1.83104100	1.92304200	-0.49562500
O	2.58479900	0.61204700	-0.56657600
O	-0.77178200	-2.53968900	-0.42321200
O	0.06186500	0.04537800	2.03120900
K	0.60138700	1.97686900	0.31436800
K	-1.99798500	-0.45950600	0.45169600
K	1.42882900	-1.48397700	0.36761900
C	-2.64745600	2.69001600	-1.28272400
C	3.69141000	0.83069300	-1.34215600
C	-1.12874000	-3.59889600	-1.21365600
C	0.07621600	0.06976300	3.40404600
C	-3.10253700	3.96957900	-0.52370800
H	-2.22051400	4.56104300	-0.24183100
H	-3.77525600	4.61436800	-1.11000100
H	-3.61668900	3.68052600	0.40194900
C	-3.92518400	1.90119200	-1.69859000
H	-4.60925800	2.47600100	-2.34108600
H	-3.63378700	0.99060500	-2.23922600
H	-4.48048800	1.60044600	-0.79828700
C	-1.91521300	3.12789200	-2.58385200
H	-1.02501800	3.71820500	-2.32479000
H	-1.57585300	2.23730800	-3.12718000
H	-2.53922000	3.73320600	-3.25902300
C	3.35049800	1.74324800	-2.55558900
H	2.98091300	2.71346200	-2.19451500
H	4.20799600	1.93293100	-3.21907900
H	2.54932500	1.28020800	-3.14478300
C	4.25674000	-0.50918600	-1.90024000
H	5.14214900	-0.38148200	-2.54154200
H	4.53860300	-1.16617500	-1.06446300
H	3.47977400	-1.01809600	-2.48594200
C	4.81717700	1.51743700	-0.51654500
H	5.07272500	0.88881500	0.34634900
H	5.73503900	1.70580500	-1.09462600
H	4.45223100	2.47838700	-0.12872400
C	0.45959300	1.48264400	3.93081500
H	-0.26520800	2.22099200	3.56120600

H	0.48449200	1.54942100	5.02867400
H	1.45341600	1.75653300	3.55083800
C	-1.32276800	-0.29575600	3.98048800
H	-1.61170400	-1.29714100	3.63255000
H	-1.35885600	-0.29413800	5.08008700
H	-2.06980000	0.42358300	3.61652200
C	1.10801500	-0.94987300	3.96777800
H	0.85033500	-1.96069200	3.62258200
H	2.11059100	-0.70406900	3.59135800
H	1.15152400	-0.96674500	5.06706200
C	-1.37164700	-4.87247200	-0.35425100
H	-1.66827600	-5.75267900	-0.94536800
H	-0.45601200	-5.12077000	0.19902000
H	-2.15866300	-4.66997600	0.38408600
C	-2.43719900	-3.29194000	-2.00063000
H	-2.29375300	-2.39010600	-2.60978800
H	-2.75650300	-4.11055700	-2.66335300
H	-3.25522900	-3.09507100	-1.29236100
C	-0.01469300	-3.91976100	-2.25250200
H	0.18145800	-3.02927600	-2.86307800
H	0.91574900	-4.17837400	-1.72671000
H	-0.26462300	-4.75453000	-2.92498300

$Na_3(OtBu)_4^-$

O	-0.76606000	-2.18988300	-0.32998100
O	0.06401900	0.00370000	1.91685600
O	-1.54595700	1.75581800	-0.28818600
O	2.26651400	0.46319500	-0.41665600
C	-1.14987500	-3.22169400	-1.15778700
C	0.11658800	-0.01942800	3.29741700
C	-2.30337800	2.57107000	-1.10000900
C	3.33090300	0.66622600	-1.26711300
C	-0.29391700	-4.48731500	-0.88012000
H	-0.39687800	-4.77571300	0.17370300
H	-0.57516600	-5.34740600	-1.50571500
H	0.76567900	-4.26404600	-1.06714900
C	-0.97486000	-2.82406600	-2.64636200
H	-1.26982600	-3.62095900	-3.34564200
H	-1.57623100	-1.93238100	-2.86266500
H	0.07467300	-2.56703700	-2.83761300
C	-2.64025900	-3.58564300	-0.91647700
H	-2.78501600	-3.86080900	0.13621200
H	-3.27160100	-2.71145000	-1.12787100
H	-2.99165500	-4.41765300	-1.54453700
C	1.14446400	-1.07566200	3.78204000
H	2.13567100	-0.83506600	3.37535300
H	1.22657700	-1.12993700	4.87750300
H	0.85331100	-2.06791500	3.41175600
C	-1.27295700	-0.37774600	3.88668100
H	-1.28159700	-0.41070200	4.98600900
H	-2.01279800	0.36616600	3.56151900
H	-1.58822600	-1.36074300	3.51216200
C	0.54044700	1.36814400	3.84654900
H	-0.17645400	2.12918600	3.51102100
H	0.58964000	1.40265400	4.94478200
H	1.53064600	1.63265600	3.45186100
C	2.86395500	0.64418000	-2.74542500
H	2.11318600	1.42787800	-2.90697300
H	3.68539600	0.79802700	-3.46141300
H	2.38677000	-0.31864700	-2.96655100
C	3.99953200	2.03776800	-0.97973200
H	4.32638800	2.07430300	0.06726000
H	4.86845800	2.24123100	-1.62311000

H	3.26784100	2.84304700	-1.13372000
C	4.40053000	-0.44252200	-1.07170600
H	4.73551000	-0.44958000	-0.02650700
H	3.95781300	-1.42386600	-1.29234700
H	5.28133900	-0.31507500	-1.71830700
C	-2.00560200	2.28555600	-2.59457200
H	-2.59506100	2.91165300	-3.28129100
H	-0.94097800	2.45702800	-2.79783800
H	-2.21666600	1.23225900	-2.81727800
C	-3.81706800	2.33511200	-0.84476400
H	-4.04463900	2.52281300	0.21246600
H	-4.46670700	2.97599800	-1.45914500
H	-4.06900200	1.28825200	-1.06455300
C	-1.99307100	4.06468900	-0.81043500
H	-2.19150900	4.28284300	0.24665000
H	-0.92947800	4.26321900	-1.00226200
H	-2.58477500	4.75841700	-1.42600400
Na	1.11027200	-1.25212400	0.34605700
Na	0.55175600	1.59794900	0.37767700
Na	-1.63069700	-0.31794400	0.45398100

N-Me-Indole

C	-0.65997000	-1.47306500	0.00003600
C	0.15148500	-0.33261200	-0.00000400
C	-0.38888200	0.98515800	-0.00002600
C	-1.78526900	1.14347500	-0.00002200
C	-2.59400200	0.01418700	-0.00001000
C	-2.03700600	-1.28114200	0.00002000
H	-0.23536700	-2.47317700	0.00006200
H	-2.22476500	2.13780600	-0.00000900
H	-3.67479400	0.12696900	-0.00000200
H	-2.69562200	-2.14541600	0.00003700
C	0.72629300	1.88868700	0.00005800
C	1.86038200	1.12059200	-0.00006600
H	2.90090000	1.41719200	-0.00009100
N	1.52953700	-0.22374500	-0.00005000
H	0.69119300	2.96943400	0.00003900
C	2.45994500	-1.33308700	0.00004000
H	2.32730100	-1.95880400	0.89078500
H	2.32691100	-1.95921700	-0.89035100
H	3.47962300	-0.94173300	-0.00028000

tBuOSiMe$_3$

C	0.07072000	-1.62134600	1.72770900
H	-0.07048300	-2.69755300	1.89167000
H	1.13346700	-1.40552300	1.89035100
H	-0.49964700	-1.09285600	2.50044900
C	-2.33834200	-1.57168300	-0.20040900
H	-2.94691200	-1.03391700	0.53560100
H	-2.70373800	-1.29665100	-1.19650700
H	-2.51639400	-2.64552600	-0.06328000
C	0.49066100	-2.12836000	-1.28153200
H	0.20290500	-1.85781900	-2.30446500
H	1.56920900	-1.96150400	-1.18381200
H	0.31220400	-3.20492400	-1.16241800
Si	-0.51264900	-1.15010000	-0.01057600
C	0.48379300	2.00458800	1.35053600
C	0.53706800	1.52696100	-0.10884500
H	-0.53294100	2.32152200	1.60520200
H	0.77620400	1.20404100	2.03790400
H	1.16010100	2.85266500	1.50964900
C	1.94600800	1.03063500	-0.46659700
C	0.12173300	2.66258800	-1.05401300

H	1.97515900	0.66254400	-1.49745200
H	2.67575700	1.84291600	-0.37278200
H	2.26362700	0.22040200	0.19968600
H	0.79544900	3.52183900	-0.95890000
H	0.14053800	2.31800500	-2.09329600
H	-0.89674900	2.99074700	-0.82250700
O	-0.44163100	0.49437700	-0.29736600

Inta

C	-1.29845800	1.70118700	-0.98968200
H	-2.12059400	2.36318200	-0.68128800
H	-0.35128400	2.22230400	-0.80311300
H	-1.41034200	1.56868100	-2.07673500
C	-1.29880500	-1.70152100	-0.98909400
H	-1.40858400	-1.56882600	-2.07635100
H	-0.35243000	-2.22353100	-0.80093200
H	-2.12215200	-2.36271100	-0.68224700
C	-2.16147300	0.00037100	1.73191600
H	-2.80117500	-0.87967200	1.89304900
H	-1.36320100	0.00137400	2.48065000
H	-2.80286100	0.87930600	1.89231500
Si	-1.52596800	0.00002200	-0.08760900
C	1.63870500	-0.00111900	-1.43250000
C	1.53036100	-0.00001300	0.11613800
H	1.15631400	-0.88697800	-1.85710800
H	1.15517300	0.88347000	-1.85845200
H	2.69110300	-0.00069100	-1.75349500
C	2.26446600	1.25806400	0.65161500
C	2.26521000	-1.25687800	0.65340600
H	2.20482200	1.27247500	1.74650500
H	3.32508100	1.29415600	0.35751900
H	1.77134300	2.16382700	0.27966300
H	3.32578000	-1.29294300	0.35914700
H	2.20579300	-1.26966100	1.74833000
H	1.77236300	-2.16339100	0.28292700
O	0.23727500	-0.00017100	0.61796400
H	-3.04983800	0.00014800	-0.61836500

TSa

H	4.35886700	0.87798000	0.42031400
C	-0.80717300	-1.45166500	0.00397600
C	0.06311900	-0.35853100	-0.00529900
C	-0.41119400	0.99574100	-0.00534300
C	-1.80171100	1.20779700	0.00911700
C	-2.67187800	0.11752700	0.02030100
C	-2.18195000	-1.20254100	0.01785500
H	-0.42593200	-2.47120200	-0.00243500
H	-2.19926900	2.22250300	0.01044900
H	-3.74804300	0.28735500	0.02916600
H	-2.88074000	-2.03760200	0.02355500
C	0.75813000	1.82430800	-0.02945300
C	1.89021600	1.02283400	-0.05164300
H	3.20163000	1.08161800	0.14100500
N	1.44018500	-0.29761100	-0.02522300
H	0.76101100	2.90975400	-0.03527900
C	2.34504300	-1.42983900	-0.02067600
H	2.08963600	-2.12979300	0.78777900
H	2.31083500	-1.98280100	-0.97200800
H	3.35509200	-1.02831800	0.14101300

TSa_C3

H	1.07636900	4.37447800	0.02817400
C	-0.76353900	-1.51299900	-0.00728400

C	0.11802500	-0.42614700	-0.01090200
C	-0.32766300	0.94007200	-0.00082300
C	-1.71493300	1.16635300	0.00520400
C	-2.60220500	0.08974000	0.00573900
C	-2.13219700	-1.23811300	-0.00005800
H	-0.40443600	-2.54203500	-0.00918000
H	-2.08697800	2.18884500	0.01140100
H	-3.67582200	0.27364500	0.01186800
H	-2.84407600	-2.06250100	0.00264600
C	0.81762000	1.83153500	-0.00004100
C	1.87787700	0.97105200	-0.00809800
N	1.49265000	-0.39474100	-0.02392400
H	0.92229700	3.20378100	0.01297800
C	2.36003700	-1.54010000	0.02174000
H	2.28940000	-2.08755600	0.97614400
H	2.13623900	-2.25182700	-0.78738700
H	3.39480600	-1.20376700	-0.10031700
H	2.94550600	1.18176200	-0.01172400

N-Me-Indole_anion

C	0.61287300	-1.45970600	0.00013200
C	-0.19350200	-0.32034400	0.00000200
C	0.35852600	1.00800000	-0.00005300
C	1.76108900	1.13267300	0.00002000
C	2.56882000	-0.00818400	0.00014600
C	2.00547300	-1.29682400	0.00020300
H	0.17434200	-2.45745700	0.00018100
H	2.22144000	2.12171700	-0.00001300
H	3.65405300	0.10094200	0.00020700
H	2.65280800	-2.17347800	0.00030700
C	-0.76738400	1.88979700	-0.00015700
C	-1.99143000	1.19562700	-0.00023300
N	-1.56601100	-0.16489000	-0.00008800
H	-0.68571000	2.97601800	-0.00020800
C	-2.48934900	-1.26706300	-0.00002900
H	-2.37651500	-1.91279100	-0.88822100
H	-2.37675700	-1.91251400	0.88839900
H	-3.49226900	-0.83206200	-0.00022700

N-Me-Indole_anion_C3

C	-0.64436900	-1.45498900	-0.01542300
C	0.16990200	-0.31723200	-0.01838100
C	-0.35148100	1.03090200	0.00131600
C	-1.75146400	1.15595200	0.01191500
C	-2.57926700	0.02898000	0.01044500
C	-2.03047800	-1.26743100	-0.00254700
H	-0.22384300	-2.46197700	-0.02183200
H	-2.18216300	2.15777200	0.02507300
H	-3.66314900	0.14921600	0.02117700
H	-2.68994100	-2.13568100	-0.00044500
C	0.71529600	2.03776800	0.00656700
C	1.81552300	1.21984100	-0.00771500
N	1.53428800	-0.19803300	-0.03887700
C	2.47306100	-1.27810900	0.03364300
H	2.46080200	-1.80316700	1.00660900
H	2.29257600	-2.03644700	-0.74628500
H	3.48311300	-0.87835900	-0.11693200
H	2.88225200	1.46078800	-0.01414600

Intb

C	1.58674500	-0.06690300	1.48686200
H	0.49310100	0.06689000	1.40250100
H	1.79453100	-0.93630600	2.12335700

H	2.00915800	0.82310300	1.97167800
C	1.61817500	1.18547700	-1.30962600
H	2.02473300	2.13609400	-0.94356800
H	1.88213200	1.08544400	-2.37002200
H	0.52362600	1.21573700	-1.21193000
C	1.38087900	-1.85277100	-1.02214100
H	1.61956900	-2.74847000	-0.43592600
H	0.29277900	-1.71487300	-1.02140100
H	1.71405800	-2.02487600	-2.05307400
Si	2.15895100	-0.30599000	-0.28976100
C	4.85706000	1.55307400	0.17692200
C	4.97807600	0.01910400	0.14180300
H	4.67097200	1.94404000	-0.82889900
H	4.03160700	1.86920900	0.82340300
H	5.77933800	2.00777300	0.56021500
C	5.18835400	-0.53321700	1.56338800
C	6.16017200	-0.38576700	-0.75478500
H	5.26097700	-1.62588400	1.53099800
H	6.10825500	-0.13683000	2.01264800
H	4.34600100	-0.26776400	2.20927000
H	7.10942500	0.00793500	-0.37005300
H	6.23001900	-1.47755900	-0.80863100
H	6.00945300	-0.00581600	-1.77113900
O	3.83079100	-0.58863500	-0.43750600
C	-5.28173800	1.07805400	-0.04101000
C	-4.01121800	0.50510700	0.05328300
C	-3.81847900	-0.91470800	0.12929200
C	-4.96045500	-1.73616900	0.10738200
C	-6.23126600	-1.16484400	0.01283900
C	-6.39568500	0.23047000	-0.06120000
H	-5.40840800	2.15838400	-0.09882400
H	-4.85458700	-2.81982300	0.16346400
H	-7.11100400	-1.80809100	-0.00449500
H	-7.39596700	0.65518100	-0.13470000
C	-2.40230500	-1.10531300	0.21654600
C	-1.71305100	0.11449900	0.19657000
N	-2.75314100	1.07381700	0.09661700
H	-1.92013000	-2.07676800	0.30014000
C	-2.52850700	2.49510900	0.05387600
H	-2.86038000	2.94441200	-0.89708600
H	-3.05515200	3.02080900	0.86718800
H	-1.45428800	2.65706000	0.16526400

TSb

C	1.45544600	0.44989500	1.63171000
H	0.39477200	0.46313900	1.88356400
H	2.00590200	-0.09699100	2.40896900
H	1.82896800	1.48368200	1.63170400
C	1.34428000	0.62435400	-1.61806900
H	1.35581900	1.70216400	-1.41080500
H	2.10674000	0.42382700	-2.38322600
H	0.35485600	0.37540000	-2.00454700
C	1.12902700	-2.20457000	-0.13465700
H	0.58035800	-2.47260000	0.77375700
H	0.44048600	-2.35232600	-0.97111400
H	1.99261100	-2.87139800	-0.24513700
Si	1.68595900	-0.40200500	-0.05348700
C	4.37825700	1.55549200	-0.43596400
C	4.56585600	0.09326900	0.01629200
H	4.06740700	1.59991300	-1.48438300
H	3.61524100	2.05976200	0.16608000
H	5.31595600	2.11665900	-0.33035900
C	5.01833200	0.06178600	1.49134000

C	5.64501900	-0.57185700	-0.86035400
H	5.12525200	-0.97741600	1.82194600
H	5.98090800	0.57241000	1.63019200
H	4.27660300	0.54643300	2.13347800
H	6.61320500	-0.06073600	-0.77563100
H	5.77345700	-1.61736000	-0.55908400
H	5.33382600	-0.56033300	-1.91090600
O	3.40145300	-0.68949000	-0.13570100
C	-4.70538100	1.29314800	0.00646800
C	-3.54164400	0.51993500	0.01204000
C	-3.57802600	-0.91290600	0.01706700
C	-4.83685900	-1.54079200	0.01699400
C	-6.00099300	-0.77020700	0.01163900
C	-5.94053600	0.63558200	0.00624100
H	-4.65824900	2.38116400	0.00190600
H	-4.90463000	-2.62874800	0.02095600
H	-6.97298100	-1.26296000	0.01140100
H	-6.86127400	1.21715800	0.00177300
C	-2.20979200	-1.33357400	0.02107300
C	-1.33672800	-0.24080800	0.01870400
N	-2.20793100	0.87939000	0.01406000
H	-1.88942300	-2.37182100	0.02611700
C	-1.77020000	2.25205400	0.01090700
H	-2.11289000	2.79334500	-0.88594100
H	-2.13955300	2.80416800	0.89027700
H	-0.67923900	2.25690700	0.02645500

Intc

C	1.17480100	0.39908000	1.67781900
H	0.19533200	0.61479900	2.11902700
H	1.71390600	-0.27093600	2.35938400
H	1.75092400	1.33331000	1.65357100
C	1.13716900	0.42614500	-1.76713300
H	1.36979300	1.49491400	-1.66748200
H	1.92982000	-0.00825600	-2.38656500
H	0.18436500	0.34785900	-2.30399700
C	1.05719700	-2.38963700	-0.08981600
H	0.56103000	-2.77667600	0.80992800
H	0.47507700	-2.74397400	-0.94993100
H	2.06409400	-2.80755600	-0.14499700
Si	1.11544200	-0.47389600	-0.05263100
C	3.98298400	1.64405400	-0.37494300
C	4.15521000	0.16056000	0.04019300
H	3.65965500	1.71717100	-1.41838300
H	3.23320400	2.14426700	0.24786000
H	4.92756300	2.19691700	-0.27090100
C	4.70110600	0.11306600	1.49159900
C	5.21353000	-0.47660400	-0.89519300
H	4.82029100	-0.93266500	1.79870500
H	5.67365600	0.61796000	1.58973400
H	3.99754200	0.58699500	2.18387600
H	6.18562100	0.03672600	-0.85039900
H	5.35980900	-1.52689200	-0.61738200
H	4.85372700	-0.45243000	-1.93059600
O	3.00152400	-0.60754500	-0.06377900
C	-4.19639000	1.40191300	0.01428500
C	-3.09902700	0.53562500	0.00806000
C	-3.25331600	-0.88395100	0.01843200
C	-4.55438700	-1.41426700	0.04529800
C	-5.65140600	-0.55354700	0.05582100
C	-5.47616900	0.84288100	0.03974900
H	-4.06435700	2.48175400	-0.00266800
H	-4.70483600	-2.49294800	0.05594600

H	-6.65931600	-0.96514100	0.07523000
H	-6.34698600	1.49584700	0.04526600
C	-1.92744800	-1.42237200	-0.00270300
C	-0.99048200	-0.39718900	-0.02353800
N	-1.74380100	0.79806600	-0.00926800
H	-1.68461100	-2.47707500	0.00133900
C	-1.22031900	2.14475000	-0.05441100
H	-1.42287200	2.62943000	-1.02111500
H	-1.66900600	2.76177900	0.73630100
H	-0.14351800	2.12023600	0.09908100

TSc

C	1.18883100	0.61459700	1.52851100
H	0.33273500	0.72412300	2.20844900
H	1.99159900	0.06804100	2.02681600
H	1.58507700	1.61148600	1.30337300
C	1.13441500	0.48793500	-1.73851400
H	1.18848900	1.58160600	-1.66007600
H	2.12743000	0.12772900	-2.01452900
H	0.38674500	0.23935700	-2.50350700
C	1.10656600	-2.18296100	-0.01733500
H	0.74716600	-2.63910400	0.91409000
H	0.63933000	-2.71391900	-0.85658600
H	2.19615600	-2.25980400	-0.07672000
Si	0.75291900	-0.32827000	-0.06727900
C	4.64518500	1.60174000	-0.12770700
C	4.60901100	0.04982000	0.03496000
H	4.29825200	1.86980900	-1.13406900
H	3.95962000	2.06391100	0.59438500
H	5.64550000	2.04082400	0.02124200
C	5.12557200	-0.29233400	1.46926600
C	5.62070800	-0.55669100	-0.98763600
H	5.09186700	-1.38050600	1.60908500
H	6.15319300	0.05310200	1.67116400
H	4.46164300	0.15838700	2.21855300
H	6.65843000	-0.20616300	-0.85848100
H	5.60898200	-1.65033000	-0.89505600
H	5.29568400	-0.30913700	-2.00664600
O	3.36918400	-0.46026200	-0.18029900
C	-4.48435400	1.31541100	0.02479200
C	-3.34062000	0.50912800	0.00916700
C	-3.41757900	-0.91518300	0.01904600
C	-4.68578300	-1.51975000	0.04674400
C	-5.82601000	-0.72091500	0.06286100
C	-5.72711600	0.68435400	0.05192100
H	-4.41158300	2.40035300	0.01587900
H	-4.77460100	-2.60453400	0.05497700
H	-6.80959500	-1.18589800	0.08400100
H	-6.63304700	1.28660700	0.06461100
C	-2.06528000	-1.38434900	-0.00331700
C	-1.20428800	-0.30122200	-0.02594400
N	-2.00543300	0.85319300	-0.01682400
H	-1.74916700	-2.41918000	-0.00118500
C	-1.54425800	2.22478100	-0.03811300
H	-1.89926500	2.74795100	-0.93652000
H	-1.90124100	2.77382800	0.84367100
H	-0.45571400	2.24081400	-0.03706500

N-Me-Indole_pro

C	-2.82273700	1.23418200	0.00976200
C	-1.63506300	0.48908600	0.01279800
C	-1.63870700	-0.93288900	-0.00152300
C	-2.86940700	-1.61371600	-0.00662500

C	-4.04690500	-0.87869600	-0.00384300
C	-4.02229900	0.53220100	0.00336000
H	-2.81419400	2.32048200	0.00854400
H	-2.89529300	-2.70063600	-0.01484200
H	-5.00410600	-1.39315000	-0.00914100
H	-4.96011300	1.08141800	0.00134300
C	-0.26641300	-1.33605200	-0.00689900
C	0.52772400	-0.20361500	0.00597000
N	-0.32094700	0.91168700	0.02837100
H	0.09957700	-2.35419000	-0.01289000
C	0.06904200	2.30607600	-0.02114600
H	-0.52580900	2.88784100	0.69116500
H	1.11866300	2.40710200	0.25663500
H	-0.07130900	2.73328700	-1.02298500
Si	2.41292200	-0.19564600	0.00091100
C	3.08569000	0.71763200	-1.51892700
H	2.80762400	1.77773100	-1.53539700
H	4.18158100	0.66688300	-1.54298600
H	2.71200400	0.26383600	-2.44424200
C	2.97746600	-1.99929200	-0.06594400
H	4.07288700	-2.05309700	-0.07503400
H	2.62637700	-2.56823100	0.80238300
H	2.61450500	-2.50467900	-0.96798000
C	3.09981200	0.60248700	1.57891100
H	2.72299500	0.08904600	2.47110000
H	4.19509600	0.53688900	1.59430800
H	2.83602200	1.66228600	1.67329700

N-Me-Indole_pro_C3

C	-3.16143900	-0.16430600	-0.00035300
C	-1.85789700	0.34417000	0.00152100
C	-0.70717800	-0.49234700	0.00238600
C	-0.89640300	-1.88517900	0.00244800
C	-2.18822100	-2.39886800	0.00045200
C	-3.31039800	-1.54714100	-0.00110400
H	-4.02757300	0.49193300	-0.00161700
H	-0.04250500	-2.55811400	0.00342400
H	-2.33818500	-3.47520900	-0.00033700
H	-4.30853100	-1.97675600	-0.00320900
C	0.46433900	0.36553400	0.00156900
C	-0.03964300	1.64888000	0.00066500
H	0.49048700	2.59313000	-0.00117000
N	-1.42019700	1.65655300	0.00120000
C	-2.27216400	2.82695300	0.00080800
H	-2.91106600	2.84901200	-0.89029000
H	-2.91313200	2.84762400	0.89044500
H	-1.64660700	3.72230000	0.00230900
Si	2.27593500	-0.09709100	0.00046200
C	2.67291600	-1.18726400	-1.49934700
H	3.72752800	-1.49012200	-1.50243100
H	2.06603700	-2.10039600	-1.50832700
H	2.47501000	-0.65426600	-2.43685100
C	2.72192400	-1.03683100	1.58554100
H	3.77708800	-1.33776000	1.58529000
H	2.55109900	-0.41584200	2.47284600
H	2.11799100	-1.94464800	1.70062900
C	3.31410100	1.48702800	-0.09269500
H	3.13415700	2.14480000	0.76628800
H	4.38391200	1.24490500	-0.09905300
H	3.10296300	2.05903000	-1.00416000

TSd

C	2.051046	-1.849166	-1.808989
Si	2.618171	-2.052508	0.024813

C	4.450684	-2.561853	0.095582
O	2.602525	0.150988	-0.027036
C	3.695395	1.043393	-0.027887
C	3.195293	2.491566	-0.254028
C	4.440700	1.021768	1.330207
C	4.696690	0.732126	-1.167471
C	2.012854	-1.797296	1.839344
K	0.511768	0.944656	1.765362
O	-0.842654	2.293249	-0.018431
C	-1.118587	3.653302	-0.016254
C	-0.509167	4.342595	-1.265583
C	-2.650843	3.907855	-0.029007
C	-0.533714	4.333812	1.250105
K	0.501736	0.905328	-1.785555
K	-2.753768	0.515718	-0.009380
O	-1.476362	-0.900297	1.814224
C	-2.089284	-1.239187	3.014399
C	-2.075768	-2.776207	3.230698
C	-3.568696	-0.766665	3.032992
C	-1.363149	-0.579155	4.217346
O	-1.478295	-0.938351	-1.806202
C	-2.088387	-1.295932	-3.002364
C	-2.068187	-2.835558	-3.198115
C	-1.363697	-0.649010	-4.213345
C	-3.569703	-0.829747	-3.028846
K	-0.777038	-2.699093	0.019348
H	-0.928044	3.896850	-2.179000
H	0.579197	4.199466	-1.278474
H	-0.705239	5.422484	-1.301545
H	-3.099736	3.458532	-0.926747
H	-2.910891	4.974588	-0.029940
H	-3.115871	3.456667	0.859690
H	-1.042624	-3.147611	3.230978
H	-2.627328	-3.275547	2.419809
H	-2.541908	-3.082309	4.176401
H	3.764549	1.325608	2.142161
H	5.297731	1.707412	1.340553
H	4.805749	0.018075	1.564245
H	5.122354	-0.268690	-1.067114
H	5.525139	1.452092	-1.185470
H	4.188442	0.782979	-2.139222
H	-0.313132	-0.898919	4.244194
H	-1.814601	-0.833958	5.185129
H	-1.395281	0.516141	4.120244
H	-3.617612	0.326170	2.920708
H	-4.093332	-1.025237	3.962182
H	-4.121352	-1.228522	2.201769
H	-4.120873	-1.281465	-2.191152
H	-4.092549	-1.104106	-3.954505
H	-3.623265	0.264444	-2.932783
H	-1.400846	0.447382	-4.131327
H	-1.812680	-0.918995	-5.178126
H	-0.312166	-0.964399	-4.234544
H	-2.617660	-3.326365	-2.380652
H	-1.033463	-3.202481	-3.193283
H	-2.532954	-3.156100	-4.139697
H	2.455660	2.787905	0.500096
H	2.727290	2.601012	-1.242081
H	4.017996	3.216269	-0.209882
H	-0.965811	3.878244	2.152509
H	-0.734390	5.412530	1.292631
H	0.555717	4.197295	1.280620
H	1.961878	-3.497211	0.033033

H	4.821753	-2.827659	-0.901640
H	5.117039	-1.798746	0.506400
H	4.540170	-3.453510	0.726750
H	2.287432	-2.800969	-2.303464
H	0.971021	-1.698013	-1.943419
H	2.584669	-1.046181	-2.328255
H	2.248128	-2.733874	2.362541
H	2.541621	-0.980999	2.343537
H	0.931848	-1.645291	1.959896

Intd

C	-2.035543	-1.893707	1.841060
Si	-2.559101	-2.008549	-0.029218
C	-4.349366	-2.657926	-0.140501
O	-2.643686	0.007856	0.034877
C	-3.753367	0.892100	0.016287
C	-3.261877	2.313941	0.371906
C	-4.396942	0.946845	-1.389252
C	-4.828752	0.510242	1.058998
C	-1.967985	-1.815724	-1.872925
K	-0.512623	0.907722	-1.797440
O	0.719410	2.308220	0.024348
C	0.943531	3.677974	0.042296
C	0.323137	4.323704	1.309543
C	2.464864	3.991996	0.043164
C	0.319488	4.356482	-1.206299
K	-0.524475	0.847403	1.809474
K	2.733794	0.623449	0.021973
O	1.537111	-0.830497	-1.818544
C	2.179419	-1.157827	-3.006283
C	2.213035	-2.695583	-3.214544
C	3.644942	-0.643530	-3.003036
C	1.454662	-0.524683	-4.224495
O	1.522453	-0.887575	1.807897
C	2.149891	-1.249587	2.993562
C	2.176707	-2.792555	3.160286
C	1.413332	-0.647697	4.220489
C	3.616980	-0.740380	3.020933
K	0.851148	-2.662170	-0.031251
H	0.767605	3.878154	2.210939
H	-0.759360	4.142612	1.331994
H	0.482089	5.408967	1.362143
H	2.940989	3.549983	0.930553
H	2.681964	5.068080	0.056217
H	2.938039	3.571382	-0.856078
H	1.191053	-3.096379	-3.229444
H	2.765278	-3.174684	-2.392104
H	2.702844	-2.992981	-4.151051
H	-3.673800	1.311902	-2.132457
H	-5.262548	1.620753	-1.413829
H	-4.728602	-0.045020	-1.708736
H	-5.283740	-0.457096	0.838945
H	-5.629258	1.260237	1.090097
H	-4.382078	0.452766	2.059006
H	0.415759	-0.877425	-4.268580
H	1.930721	-0.768509	-5.183279
H	1.450912	0.571518	-4.131005
H	3.660993	0.450858	-2.895710
H	4.192198	-0.891359	-3.922066
H	4.196546	-1.085352	-2.160384
H	4.176387	-1.160084	2.172187
H	4.153065	-1.016008	3.938627
H	3.637610	0.356541	2.944783

H	1.413193	0.450633	4.156855
H	1.878152	-0.918912	5.177417
H	0.373047	-0.998387	4.243617
H	2.735373	-3.251026	2.330426
H	1.153502	-3.190491	3.154967
H	2.657014	-3.116418	4.092900
H	-2.425622	2.625667	-0.264857
H	-2.924610	2.362876	1.416813
H	-4.061620	3.056480	0.262018
H	0.759432	3.933413	-2.120687
H	0.478878	5.442576	-1.232375
H	-0.764143	4.178756	-1.229211
H	-1.788813	-3.423497	-0.039729
H	-4.797987	-2.794495	0.850601
H	-5.015215	-2.012540	-0.722724
H	-4.332925	-3.637776	-0.630713
H	-2.293768	-2.866582	2.280127
H	-0.954529	-1.772991	2.002601
H	-2.561667	-1.112072	2.405047
H	-2.215619	-2.771943	-2.352551
H	-2.491570	-1.019221	-2.418246
H	-0.886065	-1.683429	-2.012154

TSe

C	-2.288247	-2.637597	-0.244329
Si	-2.739514	-1.240765	-1.440232
C	-1.478615	0.057022	-2.052393
C	-3.854729	-1.838996	-2.837648
O	-3.583678	-0.257350	-0.272583
C	-4.770351	0.541467	-0.290422
C	-6.007882	-0.364580	-0.405914
C	-4.802769	1.280508	1.058113
C	-4.745725	1.568556	-1.436459
K	1.261315	1.778564	-1.843300
O	0.594648	2.112739	0.668052
C	0.513407	3.390012	1.206214
C	0.526726	4.470204	0.089822
C	-0.793670	3.571196	2.023413
C	1.712068	3.668633	2.153413
K	-1.211336	0.242262	1.335872
K	2.549229	0.413420	1.303974
O	2.907089	-0.095077	-1.231298
C	4.134704	-0.221599	-1.867575
C	4.253163	0.776017	-3.053158
C	4.326805	-1.653615	-2.431623
C	5.298214	0.068972	-0.881558
O	0.777803	-1.479841	1.571655
C	0.878405	-2.370242	2.633540
C	2.088939	-2.017478	3.542852
C	1.072545	-3.823784	2.126891
C	-0.399823	-2.334424	3.515050
K	1.304747	-2.321583	-1.017287
H	-0.821992	2.852300	2.855359
H	-1.667125	3.395708	1.380418
H	-0.895429	4.574659	2.456879
H	1.713280	2.945224	2.981207
H	1.691435	4.674292	2.593484
H	2.657753	3.566745	1.601850
H	3.522273	-1.891071	-3.140259
H	4.298638	-2.386603	-1.612498
H	5.283300	-1.783883	-2.954586
H	-3.876261	2.229789	-1.345252
H	-5.647923	2.191247	-1.418825

H	-4.699498	1.074449	-2.412246
H	-6.022880	-0.889574	-1.365090
H	-6.932320	0.219549	-0.324563
H	-5.999727	-1.112681	0.394253
H	3.450099	0.591721	-3.780556
H	5.208165	0.698850	-3.588864
H	4.169139	1.810925	-2.687016
H	5.204240	1.087659	-0.478295
H	6.289869	-0.015326	-1.345515
H	5.263650	-0.640333	-0.042428
H	3.023693	-2.066480	2.965003
H	2.197756	-2.696967	4.398412
H	1.976749	-0.999080	3.943930
H	-0.541988	-1.325363	3.931160
H	-0.358268	-3.032886	4.361214
H	-1.280418	-2.591349	2.912546
H	2.003077	-3.897955	1.545198
H	0.235122	-4.112358	1.479555
H	1.137022	-4.557065	2.941619
H	-3.933529	1.943911	1.156779
H	-4.790917	0.560108	1.884732
H	-5.703604	1.897053	1.155098
H	1.471379	4.423752	-0.473193
H	0.433754	5.493006	0.477249
H	-0.305800	4.299716	-0.606785
H	-0.670728	-2.497580	-2.575768
H	-4.645686	-2.502589	-2.469266
H	-4.325698	-1.022447	-3.397398
H	-3.225247	-2.409811	-3.527247
H	-2.117937	-3.556473	-0.807433
H	-1.375648	-2.441398	0.331835
H	-3.114461	-2.781839	0.467901
H	-1.164991	-0.187760	-3.068237
H	-1.894153	1.075447	-1.992966
H	-0.585994	-0.002500	-1.420037

Inte

C	-3.071549	-0.993151	-2.851276
Si	-4.228234	0.100264	-1.852172
C	-3.889484	1.921383	-2.222285
C	-6.016504	-0.313140	-2.315691
O	-3.851050	-0.225130	-0.229980
C	-4.646819	-0.141371	0.976971
C	-5.653555	-1.301325	1.010530
C	-3.662683	-0.285435	2.145545
C	-5.360826	1.215626	1.067664
K	1.807404	1.959896	-1.494925
O	0.743023	1.793200	0.915022
C	0.505221	2.917141	1.686576
C	0.756785	4.217046	0.871835
C	-0.962027	2.943748	2.189097
C	1.437227	2.948257	2.929890
K	-0.889221	-0.171735	0.093357
K	2.538620	-0.031230	1.526404
O	3.633226	0.175379	-0.860069
C	4.992407	0.237167	-1.113421
C	5.357055	1.548238	-1.860969
C	5.445038	-0.960283	-1.993002
C	5.805955	0.195422	0.209131
O	0.987244	-1.980590	0.694109
C	0.832294	-3.190005	1.349264
C	1.682185	-3.230462	2.649130
C	1.283048	-4.371736	0.446541

C	-0.651638	-3.423996	1.738301
K	2.026581	-1.741211	-1.711176
H	-1.159310	2.048138	2.793279
H	-1.648992	2.938320	1.331942
H	-1.194282	3.824082	2.804059
H	1.263197	2.055957	3.548216
H	1.280465	3.829122	3.566836
H	2.489375	2.951205	2.610741
H	4.904031	-0.944997	-2.949753
H	5.217993	-1.905838	-1.480015
H	6.520124	-0.953176	-2.217442
H	-4.636274	2.035672	1.021540
H	-5.907878	1.297114	2.013818
H	-6.083597	1.345594	0.255418
H	-6.394862	-1.213987	0.211711
H	-6.189692	-1.317195	1.966414
H	-5.130945	-2.256895	0.894072
H	4.812160	1.596807	-2.814141
H	6.428956	1.637517	-2.083364
H	5.068615	2.416519	-1.251878
H	5.524512	1.045159	0.847168
H	6.892219	0.241960	0.052929
H	5.587800	-0.734725	0.753189
H	2.745661	-3.092983	2.405956
H	1.586528	-4.175330	3.200815
H	1.371732	-2.418780	3.322572
H	-0.992930	-2.616661	2.400709
H	-0.817725	-4.377615	2.257948
H	-1.278165	-3.417231	0.835995
H	2.340789	-4.250141	0.171406
H	0.682280	-4.387466	-0.473852
H	1.177215	-5.352386	0.929739
H	-2.946996	0.544174	2.158071
H	-3.115904	-1.232584	2.073939
H	-4.194887	-0.276783	3.103149
H	1.804275	4.256107	0.537985
H	0.561765	5.132837	1.445879
H	0.107018	4.233586	-0.014431
H	0.252565	0.061040	-2.322735
H	-6.235880	-1.378551	-2.182281
H	-6.763114	0.260293	-1.755337
H	-6.162720	-0.081214	-3.378923
H	-3.322594	-0.925193	-3.918204
H	-2.015889	-0.702611	-2.752334
H	-3.172625	-2.045007	-2.554711
H	-4.038331	2.127133	-3.290081
H	-4.545905	2.593816	-1.658232
H	-2.851119	2.181239	-1.982566

TSf

C	3.792349	-3.287794	1.183720
C	2.845585	-2.844668	0.243501
C	3.165718	-2.930804	-1.142482
C	4.385545	-3.451126	-1.592818
C	5.302868	-3.880612	-0.635983
C	5.009221	-3.798132	0.739452
C	1.523836	-2.279572	0.305418
C	1.052849	-2.030474	-0.984972
N	2.083490	-2.429830	-1.845045
C	1.999778	-2.417584	-3.290127
K	-1.800411	-2.379905	-0.204142
O	-3.913777	-0.886958	-0.948220
C	-5.108970	-1.476418	-1.329214

C	-6.247596	-1.108890	-0.339693
C	-4.981477	-3.023368	-1.360990
C	-5.533831	-1.003421	-2.746603
K	-3.566915	0.607650	1.206693
O	-2.022850	2.227833	-0.178654
C	-2.058072	3.603195	-0.000490
C	-0.794281	4.099294	0.750433
C	-3.301182	4.024176	0.831031
C	-2.128416	4.336536	-1.367635
K	-2.714859	0.964952	-2.322797
O	-1.507335	-0.829268	1.908982
C	-1.486752	-1.321986	3.207439
C	-2.719706	-0.827152	4.016793
C	-1.515954	-2.874892	3.213664
C	-0.214665	-0.856037	3.960049
K	0.176618	0.727397	0.491717
O	2.916736	1.887714	0.262660
C	3.656969	1.978777	1.508448
C	5.087801	1.445686	1.350815
Si	3.416261	2.149229	-1.332214
C	4.234867	3.840496	-1.556310
C	1.814616	2.116930	-2.328095
C	4.561969	0.791166	-1.964710
C	3.663083	3.443005	1.970962
C	2.899188	1.107256	2.517254
H	-0.183944	0.241475	3.992298
H	0.683123	-1.205706	3.436431
H	-0.168891	-1.225668	4.993518
H	-2.728710	0.272040	4.058021
H	-2.727088	-1.193334	5.051853
H	-3.651665	-1.171832	3.543784
H	-4.750943	-1.256363	-3.475423
H	-5.676888	0.087404	-2.751031
H	-6.471278	-1.458135	-3.092905
H	5.081151	0.405693	1.009916
H	5.610173	1.487145	2.313129
H	5.664405	2.046081	0.638902
H	4.225669	4.075899	1.277844
H	4.122453	3.533781	2.962162
H	2.638399	3.825900	2.029908
H	-4.196394	-3.320715	-2.070494
H	-5.909381	-3.527618	-1.661405
H	-4.711293	-3.397768	-0.363132
H	-5.990903	-1.453913	0.671678
H	-7.215099	-1.553995	-0.607627
H	-6.379556	-0.017794	-0.310105
H	-4.219136	3.675730	0.336473
H	-3.384506	5.111141	0.962713
H	-3.255204	3.575964	1.834291
H	-0.722382	3.597712	1.725483
H	-0.797890	5.182803	0.930487
H	0.109462	3.859995	0.174692
H	-3.053140	4.061451	-1.897347
H	-1.273632	4.043621	-1.991650
H	-2.119759	5.430664	-1.273974
H	2.810861	0.080762	2.145658
H	1.896611	1.508418	2.709738
H	3.424390	1.079443	3.478334
H	-2.432498	-3.234844	2.722531
H	-1.497727	-3.301127	4.225517
H	-0.650315	-3.272039	2.668187
H	-0.608346	-0.473885	-2.132858
H	3.580603	4.653119	-1.219337

H	5.186603	3.930270	-1.020031
H	4.447464	4.007004	-2.620402
H	2.024542	2.376358	-3.374065
H	1.345506	1.125425	-2.331096
H	1.084641	2.843384	-1.950677
H	4.649944	0.863500	-3.057030
H	5.573135	0.856635	-1.549475
H	4.167251	-0.203114	-1.726055
H	3.573142	-3.241078	2.248880
H	5.743211	-4.146058	1.462407
H	6.258227	-4.288929	-0.956203
H	4.614460	-3.522168	-2.653243
H	0.968190	-2.085100	1.217749
H	2.857679	-1.894771	-3.733084
H	1.973819	-3.436256	-3.702947
H	1.085353	-1.898791	-3.582972
H	-0.044459	-1.056073	-1.720930

TSf_C3

C	2.081390	-2.879926	-1.046917
C	2.990725	-3.518735	-0.147623
N	2.599295	-3.183064	1.129030
C	1.463180	-2.364201	1.017696
C	1.089227	-2.125766	-0.290715
C	3.201248	-3.665268	2.350017
C	2.278579	-3.074596	-2.427352
K	-1.848768	-2.260085	0.255030
O	-1.584684	-0.317085	2.035701
C	-1.662177	-0.522759	3.404836
C	-0.384824	-0.011410	4.119009
C	-2.877509	0.229627	4.019400
C	-1.832890	-2.031733	3.734466
K	-3.493793	1.039842	0.887339
O	-1.798880	2.199270	-0.754524
C	-1.759405	3.575451	-0.922517
C	-1.639035	3.947744	-2.425646
C	-0.548158	4.192093	-0.174684
C	-3.050320	4.239917	-0.368724
K	-2.481352	0.511789	-2.591908
O	-3.859043	-0.883103	-0.886820
C	-5.075575	-1.484424	-1.168520
C	-5.417013	-1.364572	-2.678822
C	-6.222389	-0.816332	-0.362479
C	-5.047797	-2.993172	-0.802786
K	0.263225	0.783022	0.387817
O	3.005387	1.952482	0.222310
Si	3.744955	1.659602	-1.275381
C	4.867935	0.147450	-1.236915
C	3.536793	2.506349	1.450211
C	2.568136	2.077512	2.559640
C	4.937603	1.953985	1.751237
C	3.563243	4.038721	1.345122
C	4.711720	3.164227	-1.895988
C	2.299564	1.326715	-2.437665
H	-0.258765	1.062952	3.931520
H	0.498246	-0.528635	3.723232
H	-0.408722	-0.164989	5.206613
H	-2.791465	1.308059	3.821656
H	-2.958201	0.099892	5.106762
H	-3.816279	-0.136885	3.577646
H	-4.628235	-1.838727	-3.279517
H	-5.484286	-0.304406	-2.964996
H	-6.370891	-1.837884	-2.946784

H	4.920742	0.860475	1.800696
H	5.296721	2.335884	2.713651
H	5.661717	2.255771	0.987054
H	4.272268	4.374072	0.582735
H	3.858951	4.485361	2.301707
H	2.570152	4.417114	1.080795
H	-4.261458	-3.503792	-1.376446
H	-5.995853	-3.507119	-1.009530
H	-4.833740	-3.114143	0.268791
H	-6.026430	-0.909508	0.714991
H	-7.207357	-1.259681	-0.560615
H	-6.281447	0.252648	-0.612525
H	-3.934091	3.809341	-0.860574
H	-3.077334	5.326933	-0.522232
H	-3.134687	4.061492	0.713354
H	-0.608569	3.942975	0.893856
H	-0.499287	5.285976	-0.263348
H	0.391101	3.782116	-0.568159
H	-2.523494	3.593067	-2.976594
H	-0.749777	3.469762	-2.857201
H	-1.560569	5.029242	-2.599011
H	2.489840	0.985589	2.603034
H	1.570781	2.500493	2.389979
H	2.911023	2.432576	3.537678
H	-2.752991	-2.415738	3.270080
H	-1.899871	-2.232166	4.812241
H	-0.982189	-2.603541	3.340720
H	-0.490872	-0.921748	-1.903946
H	4.079425	4.057542	-1.958183
H	5.575743	3.405196	-1.266062
H	5.094504	2.959258	-2.904191
H	2.661220	1.246587	-3.470916
H	1.799208	0.379931	-2.201812
H	1.557384	2.134076	-2.409801
H	5.202151	-0.084845	-2.256487
H	5.763477	0.288090	-0.622138
H	4.329691	-0.733089	-0.867906
H	1.016247	-2.010931	1.943547
H	0.043256	-1.323644	-1.309276
C	3.331466	-3.869284	-2.872221
H	1.604616	-2.607145	-3.142030
H	3.480994	-4.021651	-3.938624
C	4.209243	-4.487312	-1.958745
C	4.051367	-4.322353	-0.585291
H	5.022366	-5.105411	-2.331810
H	4.729193	-4.804975	0.115121
H	2.724167	-3.170984	3.200776
H	4.275154	-3.439649	2.379365
H	3.076949	-4.751163	2.466476

Intf

N	1.480090	2.443879	-1.676952
C	1.821391	3.553513	-0.913937
C	0.904139	3.602897	0.175958
C	0.033899	2.470888	-0.002099
C	0.379001	1.728850	-1.140084
C	2.846051	4.498116	-1.064120
C	2.950812	5.507098	-0.107025
C	2.054327	5.573325	0.977638
C	1.036904	4.634057	1.125100
C	2.132418	2.136962	-2.933456
K	2.538741	0.911388	0.908428
O	3.196034	-1.177762	-0.604361

C	4.496421	-1.483300	-0.973475
C	4.624496	-1.595512	-2.517136
C	4.944038	-2.838530	-0.359380
C	5.484661	-0.389607	-0.486250
K	1.139700	-1.017489	-2.233647
O	-0.260472	-2.594489	-0.719695
C	-0.980497	-3.705900	-1.129496
C	-1.046243	-3.781309	-2.679071
C	-2.431668	-3.655657	-0.583199
C	-0.320083	-5.014705	-0.615743
K	1.762208	-2.769517	0.948414
O	0.923391	-0.682221	2.268929
C	0.895965	-0.636071	3.653750
C	-0.513857	-0.247148	4.168072
C	1.264401	-2.018331	4.261419
C	1.909448	0.407491	4.199500
K	-1.139453	-0.438628	0.530109
O	-3.991618	0.311916	0.030140
Si	-4.216357	1.127888	-1.443196
C	-3.966636	2.983968	-1.221749
C	-4.901679	0.095948	1.136633
C	-4.034131	-0.360455	2.316600
C	-5.635084	1.392530	1.510619
C	-5.897073	-1.016013	0.771436
C	-5.909956	0.792763	-2.219674
C	-2.878119	0.445307	-2.575679
H	-1.250326	-0.991120	3.835855
H	-0.800435	0.729314	3.755218
H	-0.572337	-0.182672	5.263136
H	0.562582	-2.783412	3.900190
H	1.235932	-2.031097	5.359210
H	2.281588	-2.305489	3.956007
H	4.335182	-0.645464	-2.987445
H	3.956817	-2.385157	-2.891072
H	5.642301	-1.836572	-2.851686
H	-4.920655	2.183853	1.761084
H	-6.280654	1.227041	2.380497
H	-6.269315	1.746027	0.691056
H	-6.564865	-0.708024	-0.037683
H	-6.516192	-1.277670	1.637487
H	-5.357677	-1.913423	0.450359
H	5.207770	0.584532	-0.912323
H	6.527024	-0.592317	-0.766076
H	5.445973	-0.311645	0.609878
H	4.892066	-2.788561	0.737774
H	5.971362	-3.117730	-0.628868
H	4.280225	-3.644481	-0.703947
H	0.712727	-5.084685	-0.985860
H	-0.851269	-5.920756	-0.936413
H	-0.297920	-5.018912	0.483844
H	-2.411779	-3.622276	0.514901
H	-3.035917	-4.522708	-0.883379
H	-2.938158	-2.750123	-0.942212
H	-0.030661	-3.861249	-3.093992
H	-1.512714	-2.870115	-3.077471
H	-1.621427	-4.641562	-3.046960
H	-3.288089	0.400895	2.570709
H	-3.522382	-1.301272	2.080787
H	-4.648224	-0.535291	3.206722
H	2.927591	0.150344	3.871614
H	1.922080	0.463838	5.296135
H	1.661844	1.408453	3.819524
H	-6.068956	-0.275614	-2.405463

H	-6.749816	1.161543	-1.620281
H	-5.958507	1.304097	-3.190039
H	-3.034637	0.815072	-3.597888
H	-1.877476	0.773474	-2.260765
H	-2.901183	-0.650982	-2.611385
H	-4.066339	3.494423	-2.188570
H	-4.691984	3.433220	-0.534506
H	-2.958119	3.193458	-0.845657
H	0.346476	4.699901	1.963945
H	2.157640	6.373987	1.705975
H	3.734074	6.254841	-0.202266
H	3.542029	4.454643	-1.898430
H	-0.797866	2.256697	0.665076
H	2.379505	3.058689	-3.472141
H	3.061077	1.559937	-2.804194
H	1.438888	1.568572	-3.560393

TSg

N	-0.724878	2.337167	-1.435659
C	0.032580	3.175799	-0.629350
C	-0.379266	2.954015	0.717787
C	-1.390267	1.941488	0.652766
C	-1.641175	1.563886	-0.664573
C	1.044145	4.087837	-0.954655
C	1.651346	4.795935	0.087236
C	1.243894	4.606693	1.424663
C	0.234702	3.696527	1.745390
C	-0.749804	2.532911	-2.875367
K	2.362545	1.523144	1.012037
O	3.092060	0.030543	-1.018901
C	4.260660	0.279905	-1.726903
C	3.969889	0.442415	-3.243863
C	5.266843	-0.889562	-1.555470
C	4.945976	1.581231	-1.231269
K	0.842048	-0.470231	-2.237076
O	0.437303	-2.546341	-0.765173
C	0.129142	-3.837495	-1.181674
C	0.054217	-3.913862	-2.729472
C	-1.234063	-4.295420	-0.601845
C	1.210979	-4.846564	-0.707304
K	2.709835	-2.133792	0.482085
O	1.496012	-0.634965	2.236929
C	1.649932	-0.799992	3.606261
C	0.299798	-1.162345	4.280427
C	2.659219	-1.939697	3.917841
C	2.181077	0.499671	4.269608
K	-0.915653	-1.151199	1.055225
O	-3.479693	-0.151415	0.329346
Si	-3.551253	0.441671	-1.316993
C	-4.130918	2.229426	-1.764814
C	-4.503593	-0.269102	1.336268
C	-3.775624	-0.415450	2.688120
C	-5.378045	0.994544	1.383218
C	-5.361905	-1.531033	1.130749
C	-5.216682	-0.410506	-1.918630
C	-2.457656	-0.639667	-2.493009
H	-0.087380	-2.103771	3.864387
H	-0.438326	-0.370412	4.095337
H	0.381957	-1.294239	5.367481
H	2.300876	-2.888052	3.492300
H	2.814171	-2.098612	4.993222
H	3.638330	-1.706538	3.474204
H	3.262073	1.268013	-3.404198

H	3.528811	-0.481422	-3.646736
H	4.869179	0.657309	-3.835636
H	-4.758113	1.881251	1.555430
H	-6.113865	0.925795	2.193386
H	-5.922087	1.134513	0.445999
H	-5.998832	-1.455312	0.249996
H	-6.004283	-1.699675	2.004151
H	-4.715258	-2.408395	1.009882
H	4.264741	2.434973	-1.347829
H	5.871180	1.814781	-1.774344
H	5.207244	1.487353	-0.166909
H	5.525323	-1.009094	-0.493482
H	6.203349	-0.739063	-2.108402
H	4.816809	-1.827197	-1.910851
H	2.190562	-4.585196	-1.135019
H	0.991868	-5.880086	-1.005438
H	1.288735	-4.829455	0.389543
H	-1.194131	-4.290968	0.497154
H	-1.514379	-5.309350	-0.916798
H	-2.030329	-3.611783	-0.921101
H	1.018604	-3.612141	-3.164159
H	-0.723348	-3.235653	-3.102999
H	-0.175178	-4.921581	-3.100343
H	-3.095668	0.423395	2.871234
H	-3.205074	-1.353315	2.730669
H	-4.495479	-0.447213	3.513587
H	3.168009	0.758369	3.857138
H	2.296234	0.412840	5.358037
H	1.492192	1.331360	4.070084
H	-5.208739	-1.506345	-1.842392
H	-6.138152	-0.050580	-1.441617
H	-5.321264	-0.173530	-2.989876
H	-1.843030	-0.042882	-3.179055
H	-1.787775	-1.269541	-1.893166
H	-3.063941	-1.314621	-3.108166
H	-3.603053	2.591664	-2.657731
H	-5.203659	2.263019	-1.990147
H	-3.918649	2.945649	-0.964599
H	-0.079082	3.566714	2.779098
H	1.712577	5.191542	2.212585
H	2.431793	5.517287	-0.139805
H	1.349831	4.255263	-1.984162
H	-1.950501	1.576462	1.502358
H	-1.015118	3.567966	-3.125730
H	0.231188	2.327375	-3.332240
H	-1.493849	1.876945	-3.320398

Intg

N	-1.258075	2.583602	-1.443737
C	-0.511070	3.458037	-0.677586
C	-0.796074	3.175227	0.692990
C	-1.722682	2.081701	0.680332
C	-2.013727	1.711576	-0.628998
C	0.417465	4.436382	-1.057224
C	1.071662	5.147282	-0.046276
C	0.790459	4.896622	1.313443
C	-0.139783	3.925271	1.687328
C	-1.301765	2.695198	-2.891343
K	1.969245	1.809275	0.469373
O	3.040739	-0.020185	-1.199062
C	4.231960	0.307454	-1.834719
C	4.170453	-0.029551	-3.350388
C	5.419792	-0.481338	-1.219640

C	4.544661	1.821929	-1.702269
K	1.271907	-1.449981	-2.486653
O	0.761985	-2.785711	-0.362583
C	0.471759	-4.145349	-0.361276
C	0.397733	-4.697340	-1.810757
C	-0.888271	-4.423527	0.328788
C	1.567517	-4.941456	0.397964
K	2.902577	-1.806539	0.791986
O	1.490156	-0.126741	2.160655
C	1.629392	-0.021209	3.538647
C	0.254214	-0.138553	4.246519
C	2.547570	-1.146843	4.090306
C	2.260431	1.341599	3.929374
K	-0.787317	-1.011074	1.001371
O	-3.393126	-0.314102	0.270650
Si	-3.326148	0.232678	-1.407650
C	-4.435612	1.630740	-2.166888
C	-4.461382	-0.722268	1.139841
C	-3.973854	-0.462080	2.579738
C	-5.730884	0.113010	0.905527
C	-4.758275	-2.226082	0.990991
C	-4.489327	-1.193657	-2.155828
C	-1.813894	-0.518640	-2.418528
H	-0.189572	-1.125476	4.050246
H	-0.429759	0.629516	3.863729
H	0.319844	-0.020985	5.336331
H	2.136710	-2.130902	3.823460
H	2.657322	-1.117131	5.182357
H	3.556610	-1.060183	3.659505
H	3.340001	0.513530	-3.823251
H	4.013228	-1.109502	-3.494255
H	5.089184	0.235008	-3.889419
H	-5.507302	1.180058	1.012694
H	-6.504925	-0.150509	1.636255
H	-6.139753	-0.054817	-0.093015
H	-5.162288	-2.463012	0.005929
H	-5.481763	-2.553131	1.748345
H	-3.839490	-2.809834	1.129600
H	3.717674	2.415496	-2.114599
H	5.463307	2.117510	-2.225389
H	4.675019	2.093552	-0.644400
H	5.510101	-0.248225	-0.149207
H	6.383745	-0.249882	-1.691460
H	5.250068	-1.562565	-1.325971
H	2.545243	-4.795208	-0.084721
H	1.373452	-6.021663	0.426817
H	1.635055	-4.589052	1.436910
H	-0.854076	-4.087996	1.375299
H	-1.156399	-5.488149	0.334705
H	-1.691205	-3.878845	-0.184412
H	1.361170	-4.546156	-2.321422
H	-0.384978	-4.172072	-2.375240
H	0.172062	-5.770759	-1.852959
H	-3.733216	0.595998	2.724244
H	-3.080387	-1.056404	2.814519
H	-4.743484	-0.739639	3.309350
H	3.243572	1.448923	3.448265
H	2.406654	1.454400	5.011882
H	1.619411	2.166141	3.591349
H	-4.096419	-2.205654	-1.979222
H	-5.529686	-1.187895	-1.803900
H	-4.542380	-1.065548	-3.248282
H	-2.091508	-0.712209	-3.463704

H	-0.912561	0.107816	-2.402496
H	-1.583484	-1.496615	-1.969037
H	-4.480486	1.520759	-3.260115
H	-5.466265	1.498431	-1.814727
H	-4.133325	2.657171	-1.935091
H	-0.353116	3.747041	2.738845
H	1.297207	5.479467	2.078670
H	1.791619	5.916573	-0.313118
H	0.625163	4.646822	-2.103186
H	-2.173538	1.633404	1.554642
H	-1.568770	3.717036	-3.187135
H	-0.329331	2.452228	-3.343666
H	-2.052042	2.017558	-3.290437

TSh [identified from a relaxed scan of the O–Si–C_2(1-methylindole) bond angle of **Inth**; **TSh** is the maximum in the plot of *E*(B3LYP) against the O-Si-C angle.]

N	0.783886	3.075963	0.880534
C	-0.441691	3.596842	0.514279
C	-0.587564	3.390082	-0.891540
C	0.604611	2.710811	-1.310262
C	1.459629	2.519282	-0.223325
C	-1.440898	4.207957	1.283432
C	-2.608180	4.623318	0.633703
C	-2.763302	4.446386	-0.757479
C	-1.762922	3.840795	-1.520868
Si	3.254884	1.329742	-0.065814
C	3.358865	1.266481	-1.990619
C	1.297109	3.202916	2.231894
C	2.140752	0.207436	1.126991
O	4.335602	-0.135073	0.064416
C	5.699050	-0.484647	0.138671
C	5.759483	-2.017555	-0.026534
C	4.335683	2.702765	0.706666
C	6.556862	0.160902	-0.971687
C	6.282741	-0.113574	1.520264
K	-2.673608	1.260968	0.194706
O	-2.332125	-0.385716	-1.809892
C	-2.980626	-0.301789	-3.036660
C	-3.664733	-1.649462	-3.396125
C	-4.076544	0.795417	-3.010158
C	-1.977694	0.040138	-4.170111
K	-2.633108	-2.463664	-0.280594
O	-0.034902	-2.735990	-0.121432
C	0.626917	-3.917349	-0.441701
C	1.595649	-3.705792	-1.634135
C	-0.388430	-5.023972	-0.833954
C	1.456736	-4.432104	0.764666
K	-0.045025	-1.722259	2.240193
O	-2.493180	-0.859261	1.853206
C	-3.392794	-0.916628	2.910746
C	-4.387434	-2.094520	2.725321
C	-4.218916	0.392995	3.020946
C	-2.657214	-1.122582	4.263768
K	0.314604	-0.554516	-1.627729
H	-1.225771	-0.757488	-4.264221
H	-1.459685	0.980290	-3.939895
H	-2.457663	0.150978	-5.151350
H	-2.920704	-2.458298	-3.413911
H	-4.159908	-1.631770	-4.375793
H	-4.433298	-1.897344	-2.648486
H	-1.926892	-0.316619	4.420004
H	-2.124586	-2.086030	4.268009
H	-3.335879	-1.130425	5.126278

H	5.165026	-2.500494	0.757864
H	6.787303	-2.397553	0.033012
H	5.338065	-2.306097	-0.996405
H	6.187728	-0.131047	-1.961168
H	7.603850	-0.158768	-0.894844
H	6.538502	1.254270	-0.909427
H	-3.549326	1.252333	3.163701
H	-4.929776	0.382853	3.857168
H	-4.802721	0.552393	2.102383
H	-4.960691	-1.960539	1.796886
H	-5.108591	-2.185712	3.548081
H	-3.836864	-3.043838	2.658403
H	-1.077936	-5.216067	0.001460
H	0.090739	-5.977539	-1.091715
H	-0.977367	-4.703818	-1.705394
H	0.794236	-4.628684	1.621774
H	2.200946	-3.680139	1.058785
H	1.994744	-5.364408	0.549955
H	5.664117	-0.551973	2.312594
H	6.302052	0.971110	1.664361
H	7.307856	-0.487620	1.639937
H	-4.806808	0.572079	-2.218951
H	-4.626683	0.876772	-3.957006
H	-3.628173	1.774435	-2.798372
H	2.955108	0.324514	-2.393629
H	4.418104	1.252231	-2.263483
H	2.886953	2.102638	-2.514214
H	2.683991	0.094494	2.075508
H	1.132656	0.592706	1.336686
H	2.084271	-0.796823	0.689881
H	4.501312	2.535911	1.778662
H	5.325801	2.708816	0.237448
H	3.900888	3.699514	0.580611
H	-1.891030	3.721170	-2.594160
H	-3.668791	4.802559	-1.242576
H	-3.394159	5.110813	1.204713
H	-1.314570	4.372046	2.350400
H	0.836596	2.459730	-2.338183
H	1.475776	4.254901	2.488820
H	0.587676	2.787250	2.960405
H	2.236143	2.661779	2.313072
H	2.138497	-4.618619	-1.911757
H	1.033478	-3.378618	-2.521473
H	2.341447	-2.939409	-1.385258

Inth

C	-1.660280	3.994981	-1.384303
C	-0.488782	3.404691	-0.874587
C	-0.214070	3.522787	0.521409
C	-1.082635	4.188775	1.396513
C	-2.249640	4.746868	0.864144
C	-2.531979	4.654059	-0.515093
C	0.585148	2.623574	-1.416789
C	1.494377	2.282980	-0.414226
N	0.970583	2.854153	0.765031
C	1.599460	2.881796	2.073004
Si	3.314759	1.093968	-0.456756
C	2.456603	-0.053449	0.881215
O	4.740510	-0.006596	-0.498029
C	5.814929	-0.448633	0.294677
C	7.087053	-0.372666	-0.576080
C	4.309432	2.707064	-0.124002
C	3.047409	0.627194	-2.306524

C	6.044353	0.383853	1.576195
C	5.569812	-1.922948	0.689813
K	0.111372	-0.597597	-1.751942
O	-2.525898	-0.266096	-1.695373
C	-3.277473	-0.130288	-2.856823
C	-4.253607	1.070006	-2.747638
C	-2.359896	0.099702	-4.086350
C	-4.120342	-1.407788	-3.123440
K	-2.797587	-2.334660	-0.152665
K	-2.590562	1.390116	0.329716
O	-0.212387	-2.770311	-0.222041
C	0.337878	-3.993206	-0.593865
C	-0.777948	-5.021484	-0.920501
C	1.209005	-4.579466	0.549296
C	1.234043	-3.839771	-1.849949
K	0.049939	-1.776134	2.128020
O	-2.357459	-0.749807	1.963767
C	-3.163323	-0.769286	3.095805
C	-3.889663	0.588045	3.295842
C	-2.327671	-1.048236	4.375613
C	-4.245875	-1.876596	2.982135
H	-1.695296	-0.765192	-4.229017
H	-1.740066	0.992184	-3.929469
H	-2.918748	0.238514	-5.021126
H	-3.462057	-2.284276	-3.207055
H	-4.711023	-1.347973	-4.046884
H	-4.825811	-1.577112	-2.296052
H	-1.535472	-0.293745	4.478476
H	-1.860394	-2.043498	4.318654
H	-2.926989	-1.030471	5.294864
H	4.683702	-2.010958	1.329974
H	6.424336	-2.349871	1.230955
H	5.396814	-2.521890	-0.211396
H	6.944029	-0.959797	-1.489794
H	7.971756	-0.754750	-0.050110
H	7.280340	0.665173	-0.869840
H	-3.155965	1.401145	3.381764
H	-4.518047	0.609749	4.195456
H	-4.546283	0.797791	2.438551
H	-4.883436	-1.688980	2.106415
H	-4.900759	-1.933841	3.861361
H	-3.767789	-2.859022	2.858931
H	-1.417308	-5.177804	-0.039030
H	-0.384823	-6.001696	-1.220021
H	-1.404263	-4.650638	-1.744278
H	0.594468	-4.737331	1.448939
H	2.024554	-3.886755	0.796827
H	1.662651	-5.545318	0.292482
H	5.155558	0.385714	2.218278
H	6.291772	1.421785	1.335132
H	6.873628	-0.032215	2.161808
H	-4.928581	0.924492	-1.891675
H	-4.875966	1.200489	-3.642753
H	-3.693304	2.000616	-2.590307
H	2.964127	-0.464899	-2.404554
H	3.971584	0.884580	-2.835310
H	2.222280	1.112499	-2.837416
H	3.079897	-0.157647	1.778084
H	1.459560	0.289575	1.188356
H	2.384161	-1.056100	0.437017
H	4.430757	2.922721	0.945656
H	5.316399	2.609383	-0.543756
H	3.824001	3.579436	-0.574861

H	-1.884807	3.940005	-2.447053
H	-3.434383	5.116966	-0.906721
H	-2.935698	5.278199	1.518678
H	-0.858587	4.283851	2.455837
H	0.705976	2.404257	-2.471016
H	1.832727	3.911686	2.371007
H	0.942123	2.444643	2.837886
H	2.525615	2.314081	2.043562
H	1.695514	-4.784333	-2.165847
H	0.636980	-3.468985	-2.695951
H	2.043723	-3.124688	-1.653293

TSi

C	-2.117928	3.882822	-1.384434
C	-0.869044	3.458897	-0.893575
C	-0.568117	3.664751	0.485790
C	-1.485322	4.253198	1.367702
C	-2.726024	4.641960	0.855907
C	-3.036767	4.462044	-0.508905
C	0.269333	2.782972	-1.445858
C	1.229899	2.591773	-0.457114
N	0.692528	3.150543	0.716481
C	1.346840	3.267319	2.008050
Si	2.984980	1.550485	-0.482237
C	2.323656	0.319843	0.855168
O	4.687382	0.232793	-0.547233
C	5.701524	-0.264836	0.258730
C	6.970628	-0.412643	-0.617992
C	4.118077	3.029220	-0.084341
C	2.910985	1.012374	-2.316502
C	6.055192	0.640995	1.465792
C	5.327835	-1.672914	0.802815
K	0.159515	-0.605929	-1.820378
O	-2.477361	-0.454584	-1.635707
C	-3.304974	-0.371931	-2.750406
C	-4.423883	0.680453	-2.533569
C	-2.497006	0.031604	-4.011504
C	-3.986543	-1.738112	-3.036469
K	-2.516495	-2.563140	-0.109650
K	-2.597023	1.162469	0.414698
O	0.089558	-2.776503	-0.289971
C	0.723162	-3.946479	-0.703103
C	-0.320467	-5.053005	-1.010893
C	1.678006	-4.477403	0.398400
C	1.560469	-3.702641	-1.985192
K	0.361295	-1.831997	2.084019
O	-2.127906	-0.966847	2.006055
C	-2.890448	-1.065048	3.164016
C	-3.673262	0.247259	3.438819
C	-1.997123	-1.347019	4.403262
C	-3.922450	-2.219429	3.047804
H	-1.737312	-0.731705	-4.236056
H	-1.986388	0.987930	-3.838914
H	-3.122703	0.140277	-4.906977
H	-3.225320	-2.517207	-3.183224
H	-4.622359	-1.721568	-3.931175
H	-4.626394	-2.028965	-2.189624
H	-1.243188	-0.554987	4.512055
H	-1.479959	-2.312167	4.289792
H	-2.564381	-1.398213	5.341338
H	4.462733	-1.609020	1.476466
H	6.151006	-2.144591	1.357969
H	5.056977	-2.327117	-0.034648

H	6.751138	-1.065153	-1.471103
H	7.825704	-0.831697	-0.068861
H	7.258670	0.568026	-1.014275
H	-2.976708	1.093209	3.517211
H	-4.259354	0.210761	4.366026
H	-4.379649	0.449692	2.620048
H	-4.594218	-2.037264	2.196875
H	-4.546521	-2.333849	3.943617
H	-3.402942	-3.174173	2.881533
H	-0.915892	-5.271651	-0.111918
H	0.135969	-5.995447	-1.340105
H	-1.001284	-4.719539	-1.807237
H	1.110861	-4.695144	1.316743
H	2.447704	-3.728131	0.626073
H	2.193936	-5.402136	0.110149
H	5.183856	0.786124	2.118452
H	6.387337	1.626563	1.122673
H	6.857981	0.207694	2.077470
H	-5.023036	0.411838	-1.651374
H	-5.108996	0.760450	-3.387762
H	-3.985080	1.672080	-2.363483
H	2.959576	-0.081143	-2.381785
H	3.840488	1.353377	-2.782237
H	2.076347	1.400703	-2.911598
H	2.987481	0.320652	1.726233
H	1.298793	0.544897	1.190547
H	2.379951	-0.684778	0.421187
H	4.471517	3.010895	0.952333
H	5.007956	2.947117	-0.714909
H	3.635086	3.996584	-0.265504
H	-2.365675	3.758319	-2.435813
H	-4.001708	4.793611	-0.883621
H	-3.453998	5.107222	1.515222
H	-1.243997	4.412420	2.415254
H	0.385929	2.524519	-2.490749
H	1.417765	4.319385	2.308882
H	0.793158	2.722304	2.784710
H	2.353171	2.860353	1.946124
H	2.082289	-4.603427	-2.332757
H	0.907311	-3.369412	-2.805582
H	2.319554	-2.930776	-1.802355

K4(OtBu)3(tBuOSiMe3)$^+$

K	1.529650	2.469703	-0.863871
O	2.995643	0.355014	-1.126126
C	4.279103	0.522211	-1.654380
C	4.580494	-0.542707	-2.741120
C	5.348742	0.388667	-0.540652
C	4.436949	1.919939	-2.308616
K	1.740887	-1.836963	-1.730612
O	0.881902	-2.069201	0.688372
C	0.840150	-3.338453	1.270435
C	1.102221	-4.444121	0.214509
C	-0.545456	-3.612116	1.910191
C	1.916727	-3.468834	2.378448
K	2.583480	-0.198797	1.473728
O	0.591270	1.580401	1.368380
C	0.390774	2.503313	2.398156
C	-1.003505	2.319176	3.050551
C	1.464417	2.332206	3.503781
C	0.475954	3.959578	1.869309
K	-1.115888	-0.419480	1.149408
O	-3.480616	-0.087210	-0.445791

Si	-3.152996	0.420110	-2.024073
C	-3.090982	2.302424	-2.137816
C	-4.756099	-0.202837	0.260767
C	-4.406525	-0.290868	1.751644
C	-5.631570	1.030208	0.005505
C	-5.460293	-1.488616	-0.189144
C	-4.300334	-0.294225	-3.334252
C	-1.406691	-0.260883	-2.338570
H	-1.085770	1.320247	3.504057
H	-1.793390	2.429241	2.294413
H	-1.202172	3.047347	3.846125
H	1.412307	1.320058	3.929877
H	1.345411	3.041935	4.331469
H	2.469513	2.483442	3.084159
H	3.838741	-0.481259	-3.550505
H	4.552269	-1.553868	-2.307604
H	5.571197	-0.421836	-3.194874
H	-5.116095	1.947320	0.309304
H	-6.561877	0.958690	0.578675
H	-5.907403	1.116958	-1.050854
H	-5.744319	-1.441117	-1.243978
H	-6.371950	-1.650692	0.396078
H	-4.804801	-2.354561	-0.046245
H	3.681555	2.058626	-3.095317
H	5.421284	2.068308	-2.768148
H	4.317219	2.714483	-1.556253
H	5.178879	1.143964	0.239984
H	6.372911	0.522596	-0.909652
H	5.293826	-0.607639	-0.079134
H	2.918208	-3.304887	1.955275
H	1.921624	-4.454910	2.858824
H	1.744221	-2.721460	3.166115
H	-0.746027	-2.887200	2.713233
H	-0.621135	-4.611223	2.355979
H	-1.337024	-3.527422	1.151993
H	2.105749	-4.327329	-0.222090
H	0.355481	-4.385111	-0.590576
H	1.053802	-5.456519	0.632864
H	-3.852224	0.597409	2.077852
H	-3.816585	-1.191946	1.963676
H	-5.316070	-0.354179	2.357286
H	1.480041	4.166785	1.468255
H	0.287069	4.709404	2.646692
H	-0.264472	4.118002	1.072004
H	-4.305821	-1.389963	-3.319688
H	-5.335798	0.048565	-3.234847
H	-3.953975	0.020324	-4.327225
H	-1.101614	-0.053769	-3.372139
H	-0.659481	0.195291	-1.674298
H	-1.390930	-1.348391	-2.189950
H	-2.685906	2.615386	-3.109008
H	-4.082392	2.757221	-2.039279
H	-2.456622	2.730907	-1.351078

K4(OtBu)3+

K	0.021952	2.563074	-1.235827
O	1.851330	1.047197	-0.196924
C	2.987831	1.691099	0.306322
C	4.286995	0.994199	-0.175177
C	3.046703	3.168913	-0.160513
C	2.980689	1.676306	1.855919
K	0.000465	0.000174	1.427330
K	2.211317	-1.302080	-1.231290

O	-1.832419	1.079344	-0.196058
C	-2.958185	1.742321	0.306343
C	-2.945263	1.740149	1.856018
C	-4.268189	1.058160	-0.164234
C	-3.000048	3.217093	-0.172218
K	-2.232004	-1.262582	-1.232133
O	-0.017790	-2.126539	-0.196586
C	-0.030102	-3.433135	0.305292
C	1.214338	-4.227722	-0.169365
C	-1.289224	-4.204230	-0.169514
C	-0.030101	-3.420259	1.854918
H	2.184724	3.731952	0.228822
H	3.041303	3.222308	-1.258647
H	3.945179	3.691329	0.188095
H	2.087163	2.191714	2.236597
H	3.855208	2.172075	2.294090
H	2.971275	0.640948	2.225830
H	-1.332503	-4.225077	-1.267854
H	-2.203304	-3.726555	0.215090
H	-1.309578	-5.243529	0.178579
H	1.257413	-4.248886	-1.267711
H	1.214771	-5.267408	0.178229
H	2.137219	-3.767561	0.215577
H	0.867268	-2.907722	2.230309
H	-0.040171	-4.425340	2.293414
H	-0.917354	-2.890146	2.230039
H	-2.949940	0.707920	2.234693
H	-3.810687	2.252549	2.293090
H	-2.042691	2.245281	2.229044
H	-4.328367	0.029584	0.223255
H	-4.310375	1.028686	-1.262433
H	-5.169112	1.576560	0.184048
H	4.337247	-0.037596	0.205111
H	5.195626	1.499685	0.172111
H	4.323292	0.971463	-1.273679
H	-3.891243	3.752772	0.174753
H	-2.130350	3.772756	0.210510
H	-2.996528	3.261705	-1.270696

(2-indolyl)$SiMe_3$(OtBu)$^-$

C	4.554501	1.414035	0.045754
C	3.253381	0.883872	0.018598
C	3.098922	-0.535673	0.007951
C	4.196163	-1.402108	0.014215
C	5.476011	-0.843231	0.039978
C	5.651414	0.553172	0.056314
C	1.927557	1.422470	-0.002676
C	0.990484	0.397402	-0.023852
N	1.743673	-0.797940	-0.009711
C	1.220062	-2.144565	-0.054935
Si	-1.115489	0.474151	-0.052811
C	-1.174466	-0.398726	1.677715
O	-3.001571	0.607615	-0.063321
C	-4.155047	-0.160859	0.040531
C	-5.213489	0.476032	-0.894914
C	-1.137446	-0.425296	-1.767632
C	-1.057444	2.389882	-0.090350
C	-3.982410	-1.644276	-0.374648
C	-4.701020	-0.113514	1.491906
H	-3.997297	-0.587160	2.184215
H	-5.673386	-0.618765	1.590026
H	-4.820601	0.932182	1.798976
H	-5.360016	1.526289	-0.617127

H	-6.185461	-0.037524	-0.850141
H	-4.853662	0.451920	-1.930311
H	-3.232611	-2.144412	0.248201
H	-3.658962	-1.717261	-1.418056
H	-4.926890	-2.197325	-0.270719
H	-0.564350	2.777307	0.810951
H	-2.064341	2.807379	-0.148629
H	-0.472781	2.744247	-0.948682
H	-1.750544	-1.332980	1.653721
H	-0.194907	-0.614346	2.118779
H	-1.713475	0.271388	2.359260
H	-1.369678	-1.494186	-1.668308
H	-1.930413	0.009074	-2.386660
H	-0.184793	-0.346515	-2.304670
H	4.705075	2.492696	0.056624
H	6.659377	0.964626	0.075956
H	6.346747	-1.496304	0.045532
H	4.064001	-2.481931	-0.002910
H	1.685118	2.477268	0.001579
H	1.423775	-2.629636	-1.021200
H	1.667661	-2.761415	0.736550
H	0.143090	-2.119785	0.097206

(NaOtBu)4

Na	1.063577	1.063577	1.063577
O	1.185537	-1.185537	1.185537
Na	-1.063577	-1.063577	1.063577
O	-1.185537	1.185537	1.185537
O	-1.185537	-1.185537	-1.185537
O	1.185537	1.185537	-1.185537
Na	-1.063577	1.063577	-1.063577
Na	1.063577	-1.063577	-1.063577
C	-1.994043	1.994043	1.994043
C	-1.709266	1.709266	3.486814
C	-3.486814	1.709266	1.709266
C	-1.709266	3.486814	1.709266
C	-1.994043	-1.994043	-1.994043
C	-1.709266	-3.486814	-1.709266
C	-1.709266	-1.709266	-3.486814
C	-3.486814	-1.709266	-1.709266
C	1.994043	-1.994043	1.994043
C	1.709266	-1.709266	3.486814
C	3.486814	-1.709266	1.709266
C	1.709266	-3.486814	1.709266
C	1.994043	1.994043	-1.994043
C	1.709266	3.486814	-1.709266
C	1.709266	1.709266	-3.486814
C	3.486814	1.709266	-1.709266
H	-0.653763	3.717161	1.906871
H	-2.322614	4.159210	2.322614
H	-1.906871	3.717161	0.653763
H	-3.717161	0.653763	1.906871
H	-3.717161	1.906871	0.653763
H	-4.159210	2.322614	2.322614
H	-1.906871	0.653763	3.717161
H	-2.322614	2.322614	4.159210
H	-0.653763	1.906871	3.717161
H	3.717161	-0.653763	1.906871
H	3.717161	-1.906871	0.653763
H	4.159210	-2.322614	2.322614
H	3.717161	1.906871	-0.653763
H	4.159210	2.322614	-2.322614
H	3.717161	0.653763	-1.906871

H	0.653763	3.717161	-1.906871
H	2.322614	4.159210	-2.322614
H	1.906871	3.717161	-0.653763
H	1.906871	-0.653763	3.717161
H	2.322614	-2.322614	4.159210
H	0.653763	-1.906871	3.717161
H	0.653763	-3.717161	1.906871
H	2.322614	-4.159210	2.322614
H	1.906871	-3.717161	0.653763
H	-0.653763	-3.717161	-1.906871
H	-2.322614	-4.159210	-2.322614
H	-1.906871	-3.717161	-0.653763
H	-3.717161	-1.906871	-0.653763
H	-4.159210	-2.322614	-2.322614
H	-3.717161	-0.653763	-1.906871
H	-0.653763	-1.906871	-3.717161
H	-1.906871	-0.653763	-3.717161
H	-2.322614	-2.322614	-4.159210
H	0.653763	1.906871	-3.717161
H	1.906871	0.653763	-3.717161
H	2.322614	2.322614	-4.159210

TSf_Na

C	-3.970466	-3.761826	0.807284
C	-3.595499	-2.619970	0.078570
C	-4.521979	-2.065713	-0.850860
C	-5.793617	-2.616665	-1.050558
C	-6.135924	-3.746425	-0.311351
C	-5.231990	-4.314280	0.608118
C	-2.424638	-1.787178	0.005027
C	-2.626349	-0.769418	-0.929620
N	-3.914268	-0.968375	-1.433815
C	-4.553583	-0.114707	-2.413512
Na	-1.804919	0.826213	0.794786
O	-1.442148	2.965425	0.137813
C	-2.402889	3.982986	0.213552
C	-1.925334	5.088490	1.183686
C	-3.745531	3.414031	0.727413
C	-2.628417	4.608439	-1.183052
Na	0.551703	2.744444	1.067822
O	1.670726	2.165482	-0.801421
C	2.683984	2.858028	-1.482346
C	3.558583	1.874553	-2.291511
C	3.577414	3.617968	-0.474510
C	2.069199	3.886334	-2.464074
Na	-0.399822	2.335069	-1.742723
O	0.288446	0.617423	1.745450
C	0.263561	0.179964	3.080741
C	1.267727	1.000602	3.924118
C	-1.149549	0.365482	3.687016
C	0.635538	-1.317394	3.167055
Na	1.748183	0.113227	0.111112
O	3.224741	-1.746806	-0.173556
C	4.519912	-1.764037	0.493957
C	4.695547	-3.054324	1.305873
Si	2.440091	-2.951797	-1.096949
C	3.572095	-3.756463	-2.376754
C	1.080122	-1.999491	-1.980813
C	1.687265	-4.276407	0.014210
C	5.635914	-1.615306	-0.549413
C	4.526341	-0.552753	1.435328
H	1.639666	-1.486318	2.757444
H	-0.072151	-1.912907	2.578271

H	0.624188	-1.694557	4.197797
H	2.275256	0.921224	3.496303
H	1.314311	0.670724	4.969733
H	0.983997	2.063494	3.927053
H	-2.975759	3.840972	-1.887951
H	-1.687203	5.031192	-1.562509
H	-3.373440	5.414151	-1.173321
H	3.879834	-3.177118	2.025775
H	5.640071	-3.025506	1.860233
H	4.721872	-3.936712	0.657823
H	5.676178	-2.477552	-1.219803
H	6.609523	-1.527889	-0.054076
H	5.477476	-0.716467	-1.154156
H	-4.100349	2.619806	0.057959
H	-4.531774	4.176905	0.792113
H	-3.614920	2.987482	1.731910
H	-1.759656	4.661954	2.182467
H	-2.647007	5.909221	1.284408
H	-0.977790	5.517025	0.828205
H	2.981240	4.356307	0.080612
H	4.403196	4.154955	-0.958369
H	4.008139	2.916566	0.251661
H	4.033675	1.148443	-1.619521
H	4.353051	2.380855	-2.854774
H	2.936082	1.317076	-3.002333
H	1.406510	4.577965	-1.925981
H	1.485973	3.373794	-3.244219
H	2.829597	4.486374	-2.979217
H	3.724050	-0.628868	2.176914
H	4.404136	0.381124	0.872953
H	5.477398	-0.488735	1.974914
H	-1.464652	1.415085	3.604977
H	-1.191238	0.088436	4.747809
H	-1.882095	-0.264989	3.163195
H	-1.216729	0.565944	-2.536716
H	4.029231	-3.018303	-3.045324
H	4.373250	-4.357024	-1.931751
H	2.970115	-4.432623	-2.997660
H	0.619674	-2.643668	-2.740723
H	0.250439	-1.687013	-1.333809
H	1.460806	-1.116819	-2.509622
H	0.990354	-4.892596	-0.567936
H	2.435799	-4.946325	0.450678
H	1.116640	-3.826396	0.834673
H	-3.280314	-4.211505	1.518700
H	-5.528076	-5.197272	1.169449
H	-7.116492	-4.196462	-0.445510
H	-6.494701	-2.181011	-1.757965
H	-1.503550	-1.956364	0.556341
H	-4.953520	-0.706796	-3.246326
H	-5.381895	0.459285	-1.974468
H	-3.811424	0.581644	-2.807225
H	-1.713719	0.105783	-1.873805

Thiophene

S	0.000000	1.199857	0.000000
C	-1.243254	-0.011475	0.000000
C	-0.715255	-1.272902	0.000000
C	0.715261	-1.272880	0.000000
C	1.243246	-0.011458	0.000000
H	2.284590	0.281299	0.000000
H	1.319095	-2.173981	0.000000
H	-1.319074	-2.174011	0.000000

H	-2.284600	0.281274	0.000000

TSf_thiophene

S	1.394195	-3.704484	-2.204395
C	2.293233	-4.689143	-1.084296
C	2.068496	-4.266896	0.198018
C	1.169190	-3.148063	0.256828
C	0.688515	-2.688474	-0.960663
H	2.518487	-4.734789	1.070136
H	2.917501	-5.508686	-1.418423
K	-2.155223	-2.136536	-0.101111
O	-1.259416	-0.659168	1.903137
C	-1.307144	-1.109962	3.215191
C	0.091059	-1.040655	3.881072
C	-2.277949	-0.245961	4.069897
C	-1.804574	-2.579994	3.282711
K	-2.852098	1.297175	1.213513
O	-1.015516	2.322980	-0.365524
C	-0.681938	3.668792	-0.357627
C	-0.698824	4.253257	-1.797078
C	0.735704	3.886638	0.232309
C	-1.687516	4.484878	0.500627
K	-2.172577	1.154701	-2.373489
O	-3.796269	-0.133916	-0.796482
C	-5.136150	-0.349109	-1.078897
C	-5.498386	0.188672	-2.490571
C	-6.042530	0.370497	-0.044006
C	-5.475424	-1.863784	-1.043886
K	0.687677	0.305781	0.329760
O	3.607998	0.791002	0.177896
Si	4.221070	0.359431	-1.343849
C	4.839636	-1.419716	-1.369885
C	4.286584	1.143887	1.408510
C	3.244640	0.992654	2.524209
C	5.469946	0.203630	1.681691
C	4.752127	2.605348	1.327657
C	5.591783	1.524428	-1.932267
C	2.743753	0.543360	-2.500044
H	0.455873	-0.005177	3.871594
H	0.805260	-1.658581	3.322223
H	0.087618	-1.388411	4.923007
H	-1.952946	0.804725	4.061257
H	-2.327064	-0.566089	5.119009
H	-3.298983	-0.303528	3.663761
H	-4.884297	-0.313593	-3.251493
H	-5.303414	1.270098	-2.541695
H	-6.551864	0.031899	-2.757585
H	5.138456	-0.839537	1.712258
H	5.929353	0.445362	2.646795
H	6.246536	0.298347	0.915103
H	5.515603	2.738358	0.556048
H	5.178970	2.927025	2.284802
H	3.905494	3.258366	1.090989
H	-4.858400	-2.402724	-1.776571
H	-6.527540	-2.077293	-1.274116
H	-5.267297	-2.271488	-0.044259
H	-5.826753	-0.004089	0.966366
H	-7.114761	0.225218	-0.231698
H	-5.845317	1.451934	-0.061723
H	-2.707394	4.351200	0.112306
H	-1.472961	5.561848	0.511755
H	-1.663930	4.134370	1.542738
H	0.771659	3.499516	1.259968

H	1.032166	4.944003	0.261639
H	1.481185	3.343809	-0.363434
H	-1.710591	4.180415	-2.224515
H	-0.009543	3.685773	-2.436914
H	-0.404864	5.310384	-1.839356
H	2.869552	-0.035546	2.569711
H	2.401759	1.675172	2.362087
H	3.680194	1.235080	3.499819
H	-2.819454	-2.654182	2.864120
H	-1.844358	-2.973844	4.307038
H	-1.139025	-3.230656	2.700638
H	-0.567509	-0.777924	-1.991271
H	5.257151	2.568059	-1.954794
H	6.497391	1.472633	-1.317394
H	5.880993	1.249202	-2.954972
H	3.073586	0.436292	-3.541501
H	1.980036	-0.224986	-2.332302
H	2.276395	1.531563	-2.403367
H	5.059281	-1.717467	-2.403434
H	5.756339	-1.558735	-0.786007
H	4.080968	-2.112110	-0.987053
H	0.875800	-2.697604	1.204694
H	-0.105011	-1.488086	-1.595773

Furan

O	1.106354	-0.351163	0.000000
C	0.662601	0.938539	0.000000
C	-0.697986	0.974420	0.000000
C	-1.132227	-0.393538	0.000000
C	0.000000	-1.148818	0.000000
H	0.190850	-2.211138	0.000000
H	-2.149482	-0.759870	0.000000
H	-1.317717	1.860385	0.000000
H	1.431193	1.696310	0.000000

TSf_furan

O	1.685307	-2.634999	-2.539554
C	2.347806	-3.810902	-2.339158
C	2.036226	-4.328872	-1.120864
C	1.112012	-3.394701	-0.534315
C	0.899608	-2.349058	-1.416062
H	2.410444	-5.252671	-0.697626
H	2.987856	-4.143051	-3.145022
K	-2.047862	-2.069579	-0.790103
O	-1.385816	-1.244519	1.616041
C	-1.472911	-2.012095	2.768377
C	-0.091668	-2.131913	3.462015
C	-2.461525	-1.380239	3.789677
C	-1.984067	-3.442924	2.446618
K	-2.945399	0.831010	1.382663
O	-0.976964	2.258033	0.375109
C	-0.654426	3.494226	0.914411
C	-0.553257	4.573645	-0.197177
C	0.704224	3.438177	1.661829
C	-1.735619	3.957088	1.930619
K	-1.888679	1.762240	-1.992370
O	-3.638346	0.075103	-1.053136
C	-4.940272	-0.039899	-1.513869
C	-5.175579	0.879093	-2.743536
C	-5.955697	0.364134	-0.410893
C	-5.251358	-1.499845	-1.941495
K	0.700837	0.089363	0.535709
O	3.636449	0.467198	0.185491

Si	4.087977	1.028551	-1.347578
C	4.632140	-0.360495	-2.499698
C	4.443040	-0.035575	1.280705
C	3.512032	-0.909928	2.130801
C	5.614516	-0.887871	0.771723
C	4.950666	1.154905	2.107716
C	5.428545	2.361041	-1.245138
C	2.515533	1.798082	-2.047303
H	0.275580	-1.132024	3.731208
H	0.634445	-2.587900	2.777858
H	-0.120914	-2.737094	4.378355
H	-2.129432	-0.367061	4.058880
H	-2.545387	-1.957247	4.720109
H	-3.470093	-1.317268	3.354038
H	-4.480255	0.608956	-3.550655
H	-4.997859	1.928480	-2.465646
H	-6.195171	0.813766	-3.145934
H	5.251085	-1.724160	0.166578
H	6.176898	-1.296247	1.618945
H	6.312152	-0.295733	0.169642
H	5.647046	1.771378	1.531220
H	5.470751	0.806977	3.007872
H	4.110349	1.785646	2.417770
H	-4.558644	-1.813245	-2.735190
H	-6.273349	-1.632119	-2.320539
H	-5.128392	-2.175748	-1.082919
H	-5.829587	-0.282963	0.468532
H	-7.002098	0.285932	-0.734791
H	-5.779603	1.404735	-0.102815
H	-2.718404	4.000415	1.439389
H	-1.532302	4.948791	2.356118
H	-1.795300	3.247973	2.769301
H	0.654895	2.688953	2.464295
H	0.985796	4.397743	2.116302
H	1.506071	3.147448	0.970726
H	-1.522279	4.680217	-0.707274
H	0.196719	4.273150	-0.940689
H	-0.272571	5.564346	0.184741
H	3.070152	-1.706510	1.522069
H	2.709579	-0.309846	2.577116
H	4.062023	-1.374866	2.956441
H	-2.979740	-3.388805	1.982309
H	-2.068698	-4.081160	3.336402
H	-1.301815	-3.939524	1.744291
H	-0.320963	-0.264970	-2.116795
H	5.122938	3.189506	-0.595341
H	6.387832	1.980222	-0.876086
H	5.609522	2.775686	-2.245352
H	2.738051	2.277850	-3.009625
H	1.744114	1.040617	-2.235254
H	2.098275	2.565249	-1.384331
H	4.771141	0.040891	-3.512448
H	5.574050	-0.831719	-2.200380
H	3.859423	-1.135813	-2.554806
H	0.660865	-3.484641	0.447807
H	0.119215	-1.022879	-1.826300

N-Me-pyrrole

N	0.625625	-0.000021	-0.040981
C	-0.175263	-1.119659	-0.014824
C	-1.491750	-0.711824	0.016533
C	-1.491684	0.711890	0.016562
C	-0.175170	1.119672	-0.014827

H	0.263151	2.108061	-0.023898
H	-2.355964	1.362567	0.022847
H	-2.356066	-1.362447	0.022751
H	0.263043	-2.108052	-0.023758
C	2.074161	0.000015	0.027339
H	2.465749	0.882418	-0.486395
H	2.434419	0.007444	1.063808
H	2.464526	-0.890405	-0.473185

TSf_N-Me-pyrrole

N	1.340513	-3.541881	-1.643042
C	2.141761	-4.401021	-0.919040
C	1.971835	-4.111076	0.417648
C	1.025461	-3.041851	0.478627
C	0.618248	-2.681949	-0.817955
H	2.470194	-4.605902	1.243515
H	2.757352	-5.144426	-1.411051
C	1.171065	-3.628656	-3.081085
K	-2.149932	-2.114102	0.079027
O	-1.285917	-0.489640	1.980750
C	-1.359095	-0.842490	3.321379
C	0.035677	-0.771860	3.993835
C	-2.307460	0.112500	4.101567
C	-1.906906	-2.286471	3.491141
K	-2.825957	1.422305	1.125419
O	-0.969189	2.256952	-0.539137
C	-0.581107	3.585509	-0.622364
C	-0.568759	4.069251	-2.098884
C	0.841576	3.787942	-0.039126
C	-1.555791	4.499936	0.170548
K	-2.210858	1.030640	-2.454471
O	-3.792590	-0.150799	-0.769031
C	-5.136135	-0.397337	-1.002575
C	-5.515412	-0.059296	-2.470523
C	-6.028581	0.462341	-0.066737
C	-5.480526	-1.890875	-0.752801
K	0.706107	0.253794	0.331913
O	3.653268	0.696857	0.203718
Si	4.280096	0.170007	-1.279079
C	4.892108	-1.609979	-1.201466
C	4.315093	1.095975	1.429324
C	3.251064	1.008355	2.530584
C	5.480781	0.154980	1.767533
C	4.802592	2.545689	1.288973
C	5.656070	1.297931	-1.925692
C	2.809904	0.272721	-2.454750
H	0.433838	0.248307	3.915872
H	0.732499	-1.449557	3.485204
H	0.012863	-1.045753	5.057451
H	-1.947976	1.148818	4.021020
H	-2.376018	-0.129705	5.170363
H	-3.326795	0.058731	3.690235
H	-4.906707	-0.659178	-3.161458
H	-5.324926	1.005523	-2.671493
H	-6.571487	-0.252021	-2.701280
H	5.135937	-0.881888	1.835705
H	5.921950	0.433478	2.731210
H	6.275198	0.209060	1.015193
H	5.580116	2.631582	0.524507
H	5.219027	2.905547	2.237091
H	3.969628	3.198824	1.008271
H	-4.886115	-2.530588	-1.420598
H	-6.539175	-2.125501	-0.925609

H	-5.248488	-2.159963	0.287523
H	-5.806554	0.226780	0.983537
H	-7.103256	0.299714	-0.223972
H	-5.824895	1.529852	-0.232575
H	-2.579553	4.378274	-0.211552
H	-1.299318	5.565748	0.104962
H	-1.548075	4.225884	1.235515
H	0.858932	3.467400	1.011590
H	1.177400	4.833215	-0.076526
H	1.569182	3.180606	-0.592988
H	-1.581416	4.009257	-2.526607
H	0.097718	3.430506	-2.694005
H	-0.231180	5.108000	-2.212521
H	2.859809	-0.011375	2.612021
H	2.421308	1.694892	2.323543
H	3.672254	1.286464	3.503012
H	-2.918717	-2.358489	3.064626
H	-1.972276	-2.599250	4.541803
H	-1.256755	-3.001604	2.970653
H	-0.633778	-0.933925	-2.216001
H	5.323599	2.339490	-2.005805
H	6.558153	1.278329	-1.303677
H	5.950421	0.967631	-2.930487
H	3.142660	0.098951	-3.486269
H	2.056002	-0.490850	-2.228501
H	2.331631	1.259743	-2.426716
H	5.145752	-1.953719	-2.213398
H	5.789118	-1.726843	-0.583675
H	4.116919	-2.280450	-0.810840
H	0.670906	-2.574652	1.393015
H	2.126219	-3.868855	-3.561970
H	0.442763	-4.403034	-3.362415
H	0.817071	-2.668889	-3.462899
H	-0.211093	-1.539788	-1.699384

Pyridine

N	0.000000	0.000000	1.421094
C	0.000000	-1.142285	0.721852
C	0.000000	-1.198677	-0.673006
C	0.000000	0.000000	-1.385671
C	0.000000	1.198677	-0.673006
C	0.000000	1.142285	0.721852
H	0.000000	-2.059684	1.309018
H	0.000000	-2.157813	-1.182643
H	0.000000	0.000000	-2.472530
H	0.000000	2.157813	-1.182643
H	0.000000	2.059684	1.309018

TSf_pyridine

C	-5.371307	-1.953231	-1.958406
Si	-4.149988	-0.588496	-1.480443
C	-4.862727	1.095921	-1.947004
O	-3.702222	-0.674430	0.147326
C	-4.487975	-0.745973	1.359860
C	-3.545359	-0.330733	2.497595
C	-5.684661	0.214600	1.304615
C	-4.960231	-2.191801	1.574695
C	-2.535293	-0.843883	-2.417666
K	-0.741713	0.012889	0.480544
O	1.446741	0.954338	1.784476
C	1.394985	1.707273	2.947310
C	-0.052561	1.778100	3.499953
C	2.302953	1.086927	4.044320

C	1.879784	3.160697	2.689149
K	2.782778	-1.211572	1.432894
O	0.809187	-2.246988	0.006816
C	0.368978	-3.537661	0.256925
C	0.196923	-4.334784	-1.065745
C	-0.995092	-3.527886	0.994816
C	1.383421	-4.310854	1.145983
K	2.032104	-1.575783	-2.170587
O	3.811328	-0.256808	-0.809513
C	5.159388	-0.203812	-1.124762
C	5.440074	-0.908040	-2.480415
C	6.009766	-0.906786	-0.032505
C	5.644865	1.266669	-1.239999
K	2.343313	1.941515	-0.462357
C	-0.493125	2.502249	-1.400371
N	-1.417328	2.581347	-0.392147
C	-2.136028	3.706230	-0.230157
C	-0.338941	3.618213	-2.251868
C	-1.073969	4.790592	-2.075202
H	-0.418661	0.764382	3.714050
H	-0.713227	2.234450	2.751812
H	-0.130496	2.365122	4.425509
H	1.964550	0.066876	4.277128
H	2.302341	1.658714	4.982160
H	3.341312	1.034697	3.685998
H	4.856181	-0.428577	-3.278482
H	5.146282	-1.966472	-2.420955
H	6.497431	-0.876825	-2.774975
H	-5.350599	1.240661	1.119687
H	-6.229084	0.196495	2.255530
H	-6.389706	-0.068728	0.515561
H	-5.648362	-2.506541	0.784494
H	-5.481583	-2.287510	2.534397
H	-4.104051	-2.874152	1.578156
H	5.085436	1.785659	-2.031386
H	6.713283	1.353264	-1.478369
H	5.473952	1.791306	-0.289147
H	5.864196	-0.407203	0.935643
H	7.086123	-0.901881	-0.250593
H	5.692976	-1.954506	0.067926
H	2.371921	-4.325283	0.665026
H	1.087552	-5.351619	1.333860
H	1.480175	-3.818625	2.124897
H	-0.894645	-2.987779	1.946496
H	-1.370341	-4.535979	1.218916
H	-1.751184	-3.011802	0.390236
H	1.164979	-4.428638	-1.581649
H	-0.498698	-3.807524	-1.731744
H	-0.187228	-5.351957	-0.911837
H	-3.170221	0.686305	2.338506
H	-2.695152	-1.019859	2.562814
H	-4.063916	-0.354047	3.462546
H	2.920520	3.152053	2.331865
H	1.847059	3.793110	3.586480
H	1.248015	3.633114	1.924777
H	0.855686	0.673917	-2.567707
H	-4.979479	-2.948576	-1.718451
H	-6.345736	-1.847829	-1.467453
H	-5.550621	-1.920993	-3.040968
H	-2.739814	-0.987719	-3.486492
H	-1.874197	0.027066	-2.333170
H	-1.996377	-1.730327	-2.061601
H	-4.940802	1.170116	-3.039772

H	-5.860616	1.276717	-1.533592
H	-4.199232	1.900250	-1.609425
H	0.369996	3.549274	-3.080980
H	0.348818	1.240706	-2.078029
C	-2.001174	4.838225	-1.032529
H	-0.939870	5.648334	-2.733683
H	-2.606782	5.721112	-0.846037
H	-2.856607	3.702431	0.589481

PhCN

C	0.000000	0.000000	2.045181
C	0.000000	0.000000	0.610165
C	0.000000	1.217235	-0.091218
C	0.000000	1.210726	-1.484030
C	0.000000	0.000000	-2.180923
C	0.000000	-1.210726	-1.484030
C	0.000000	-1.217235	-0.091218
H	0.000000	2.152911	0.458415
H	0.000000	2.151889	-2.025945
H	0.000000	0.000000	-3.267340
H	0.000000	-2.151889	-2.025945
H	0.000000	-2.152911	0.458415
N	0.000000	0.000000	3.208406

TSf_PhCN

C	-3.400774	3.905276	-0.856175
C	-2.979867	3.375891	-2.090939
C	-1.889825	2.506914	-2.126710
C	-1.166416	2.118640	-0.980684
C	-1.620962	2.677956	0.235492
C	-2.710286	3.550952	0.315205
K	1.787637	2.349036	-0.288952
O	1.382483	0.899271	1.862235
C	1.381743	1.409446	3.154009
C	1.512687	2.956882	3.141039
C	0.074125	1.036741	3.897376
C	2.571207	0.845490	3.982125
K	3.359650	-0.683546	1.199247
O	1.710123	-2.242751	-0.136266
C	1.698526	-3.613529	0.081002
C	2.927267	-4.053592	0.924069
C	1.743570	-4.387493	-1.264586
C	0.419800	-4.044347	0.846055
K	2.449012	-1.084805	-2.328244
O	3.777874	0.717941	-1.002694
C	5.004554	1.213622	-1.419353
C	4.984782	2.764553	-1.481393
C	5.364745	0.683092	-2.833821
C	6.133141	0.784965	-0.443682
K	-0.385612	-0.611130	0.501676
O	-3.198200	-1.577574	0.237245
C	-3.980466	-1.564990	1.459959
C	-4.053532	-2.993711	2.017343
Si	-3.648138	-1.939397	-1.354952
C	-2.013237	-2.048014	-2.288593
C	-4.532700	-3.606139	-1.487590
C	-4.698777	-0.583486	-2.138175
C	-3.225173	-0.656223	2.437799
C	-5.386451	-0.997299	1.219312
H	-0.025084	-0.056173	3.947947
H	-0.793126	1.431835	3.354203
H	0.036798	1.426433	4.923572
H	2.507183	-0.251175	4.036611

H	2.593318	1.223787	5.012468
H	3.527934	1.122012	3.514049
H	4.586555	0.975527	-3.552807
H	5.431912	-0.414975	-2.817452
H	6.324076	1.062975	-3.209065
H	-5.331650	0.010804	0.796552
H	-5.936689	-0.941363	2.165099
H	-5.966789	-1.630727	0.539809
H	-4.611001	-3.653714	1.346185
H	-4.553238	-3.002047	2.992992
H	-3.045694	-3.404212	2.143190
H	4.210066	3.102703	-2.184091
H	5.939662	3.197249	-1.807327
H	4.759533	3.176485	-0.487098
H	5.922479	1.168276	0.564592
H	7.124640	1.153106	-0.738808
H	6.186212	-0.311945	-0.392952
H	3.856451	-3.749331	0.421204
H	2.974512	-5.138869	1.083319
H	2.896490	-3.579722	1.916147
H	0.368093	-3.514935	1.807568
H	0.385213	-5.122129	1.054333
H	-0.475716	-3.787626	0.265200
H	2.676710	-4.158941	-1.801666
H	0.898636	-4.085604	-1.897500
H	1.699250	-5.477568	-1.139682
H	-3.088472	0.342214	2.008512
H	-2.243305	-1.075989	2.687586
H	-3.777853	-0.551359	3.377796
H	2.454157	3.250358	2.653338
H	1.513434	3.397726	4.146647
H	0.679389	3.402597	2.582363
H	0.445012	0.521415	-2.115034
H	-3.928055	-4.418049	-1.066569
H	-5.508103	-3.619114	-0.988099
H	-4.710097	-3.841607	-2.545036
H	-2.202827	-2.370262	-3.320894
H	-1.502297	-1.078883	-2.344043
H	-1.328787	-2.777019	-1.838517
H	-4.797556	-0.775124	-3.214921
H	-5.709912	-0.523854	-1.722819
H	-4.224264	0.397688	-2.020991
H	-1.110250	2.433506	1.170018
H	-0.076335	1.059422	-1.624495
H	-3.030910	3.963946	1.269266
C	-4.521870	4.795946	-0.793616
H	-3.512500	3.653784	-2.997654
H	-1.586925	2.107930	-3.099962
N	-5.434645	5.517170	-0.741645

TSj_pyridine

N	1.874262	-2.218416	-1.521428
C	2.848090	-2.123421	-0.522461
C	2.750437	-3.026688	0.623986
C	1.687296	-3.878815	0.751903
C	0.686037	-3.931127	-0.257433
C	0.866613	-3.083064	-1.349524
O	2.771349	-0.504563	0.126212
C	4.005449	0.222687	0.118842
C	5.148535	-0.555272	0.810244
H	-0.074991	-4.709119	-0.268893
C	3.774262	1.521789	0.911954
C	4.417522	0.597034	-1.323578

K	0.752277	0.362836	-1.838824
O	0.134024	2.284407	-0.020987
C	0.276829	3.652886	-0.206249
C	-1.092037	4.338101	-0.490833
C	0.875957	4.326733	1.056510
C	1.202781	3.954803	-1.415236
K	-2.347462	1.443750	0.126942
O	-1.875632	-0.377316	-1.687762
C	-2.609956	-0.511944	-2.856831
C	-1.719362	-0.276965	-4.106363
C	-3.774410	0.515200	-2.900173
C	-3.224821	-1.934098	-2.967200
K	-1.800787	-2.184468	0.172122
O	-1.674501	-0.332080	1.974169
C	-2.282704	-0.445214	3.216429
C	-3.438201	0.581928	3.359268
C	-1.266407	-0.185368	4.360915
C	-2.874669	-1.866438	3.417769
K	0.834661	0.496633	1.774581
H	0.760894	3.548920	-2.336945
H	2.181515	3.481998	-1.267442
H	1.367780	5.028985	-1.573913
H	-1.570538	3.884323	-1.370768
H	-0.996067	5.413758	-0.687748
H	-1.764133	4.231261	0.374405
H	-2.079020	-2.619906	3.334999
H	-3.631997	-2.071497	2.646447
H	-3.359363	-1.998792	4.393905
H	4.837540	-0.863443	1.815076
H	6.038559	0.078505	0.907431
H	5.444797	-1.452298	0.258175
H	4.508611	-0.289651	-1.958915
H	5.379474	1.124233	-1.340338
H	3.671522	1.263511	-1.776123
H	-0.437738	-0.904515	4.296936
H	-1.709902	-0.277495	5.360900
H	-0.856613	0.831706	4.276672
H	-3.048231	1.602999	3.243597
H	-3.946909	0.528236	4.330829
H	-4.193350	0.408870	2.579099
H	-4.442084	0.362328	-2.039698
H	-4.384194	0.439524	-3.810239
H	-3.375207	1.538198	-2.852627
H	-1.297282	0.738070	-4.078755
H	-2.268232	-0.378295	-5.051911
H	-0.891978	-0.999338	-4.122185
H	-3.895520	-2.119995	-2.114771
H	-2.428373	-2.690702	-2.955957
H	-3.811810	-2.082112	-3.883194
H	3.613865	1.304234	1.977928
H	2.903814	2.058753	0.522529
H	4.643834	2.187809	0.848356
H	0.236218	4.114704	1.924130
H	0.965210	5.417154	0.959676
H	1.874975	3.926295	1.266362
H	3.554566	-3.025677	1.354598
H	1.637381	-4.556332	1.603520
H	0.156920	-3.121857	-2.181135
H	3.845764	-2.000756	-0.940307

Intj_pyridine

N	1.533826	-1.504037	-1.365480
C	2.644903	-1.725199	-0.443970

C	2.246716	-2.680366	0.649802
C	1.605612	-3.814029	0.232102
C	1.085366	-3.882896	-1.101536
C	0.974984	-2.654442	-1.766485
O	3.069818	-0.464844	0.124305
C	4.349255	0.076946	-0.284097
C	5.498014	-0.850861	0.148208
H	0.605824	-4.777104	-1.487009
C	4.456414	1.405579	0.475079
C	4.379959	0.338659	-1.798442
K	-0.015375	0.598393	-2.234647
O	-0.137836	2.339342	-0.260402
C	0.035232	3.705092	-0.420347
C	-1.321238	4.454527	-0.306516
C	0.985907	4.275765	0.665883
C	0.642729	4.028024	-1.812366
K	-2.460110	1.327739	0.506029
O	-2.268812	-0.477250	-1.372014
C	-3.315106	-0.858665	-2.196409
C	-2.952188	-0.641924	-3.690930
C	-4.592110	-0.029133	-1.889194
C	-3.660781	-2.359788	-1.999707
K	-1.104612	-2.150872	0.338671
O	-1.200690	-0.261392	2.170139
C	-1.576735	-0.484698	3.485497
C	-2.822826	0.366038	3.852763
C	-0.431239	-0.104782	4.462507
C	-1.930128	-1.978592	3.716591
K	1.087740	0.787302	1.463374
H	-0.040218	3.695441	-2.607946
H	1.598299	3.499866	-1.933175
H	0.828107	5.099332	-1.966686
H	-2.025930	4.068137	-1.056386
H	-1.231062	5.537980	-0.460431
H	-1.755459	4.301263	0.692409
H	-1.060117	-2.610411	3.490335
H	-2.756429	-2.273767	3.054034
H	-2.239391	-2.195019	4.747813
H	5.439048	-1.048595	1.224141
H	6.466181	-0.383004	-0.064321
H	5.469356	-1.809755	-0.377197
H	4.237600	-0.583617	-2.368630
H	5.342488	0.774894	-2.090590
H	3.585915	1.039268	-2.079464
H	0.465105	-0.699269	4.237153
H	-0.687188	-0.274131	5.516869
H	-0.180809	0.960306	4.350596
H	-2.599688	1.433871	3.716156
H	-3.154062	0.225112	4.890201
H	-3.663623	0.099743	3.196290
H	-4.894695	-0.181699	-0.843140
H	-5.447206	-0.297916	-2.523634
H	-4.388817	1.040768	-2.039820
H	-2.731551	0.420186	-3.871969
H	-3.756283	-0.934084	-4.379412
H	-2.061664	-1.231591	-3.949572
H	-3.950103	-2.543256	-0.954730
H	-2.785164	-2.981517	-2.231516
H	-4.488823	-2.699609	-2.635961
H	4.409820	1.236579	1.558247
H	3.647111	2.086442	0.186349
H	5.406455	1.904154	0.254588
H	0.581570	4.055907	1.663932

H	1.125454	5.362568	0.592074
H	1.976668	3.807961	0.584681
H	2.618460	-2.538129	1.661272
H	1.420386	-4.633693	0.927708
H	0.277381	-2.574964	-2.608263
H	3.498778	-2.137425	-1.018547

TSj_PhCN

C	3.461794	-1.219841	2.365338
C	4.122676	-0.001134	2.067405
C	3.462029	1.217405	2.366467
C	2.135716	1.224375	2.747126
C	1.434710	-0.001248	2.910659
C	2.135491	-1.226882	2.746002
O	3.984038	-0.000854	-0.148261
C	5.134876	0.000456	-0.923954
C	5.989507	1.265402	-0.653439
C	0.041686	-0.001174	3.136586
N	-1.128078	-0.001095	3.239774
C	4.729552	0.000692	-2.421346
C	5.991635	-1.263265	-0.654425
K	1.448447	-0.000124	-0.364690
O	-0.562684	1.870612	-0.729486
C	-0.253224	3.073404	-1.352872
C	-0.761873	3.077853	-2.820860
C	-0.919369	4.272333	-0.620256
C	1.276066	3.319984	-1.371852
K	-1.999777	0.000581	-1.880001
O	-0.563057	-1.870307	-0.730281
C	-0.254080	-3.072878	-1.354324
C	1.275192	-3.319531	-1.374316
C	-0.763610	-3.076744	-2.822008
C	-0.919840	-4.272063	-0.621782
K	-2.203852	-1.897131	1.277323
O	-3.620488	0.000164	0.218105
C	-5.006770	0.000499	0.147430
C	-5.480347	0.000892	-1.329929
C	-5.595362	1.256384	0.844145
C	-5.595935	-1.255394	0.843646
K	-2.203292	1.896598	1.278225
H	1.784253	2.535182	-1.947699
H	1.674307	3.297891	-0.349609
H	1.547272	4.283926	-1.822650
H	-0.301594	2.248379	-3.376260
H	-0.526955	4.005867	-3.358607
H	-1.854416	2.949939	-2.844568
H	-5.293937	-1.274892	1.900455
H	-5.220081	-2.166059	0.355262
H	-6.692640	-1.293190	0.811283
H	5.384909	2.163023	-0.830152
H	6.881784	1.316308	-1.292031
H	6.327025	1.289673	0.390598
H	6.329199	-1.287808	0.389592
H	6.884009	-1.312232	-1.293039
H	5.388513	-2.161739	-0.831836
H	-5.293353	1.275314	1.900962
H	-6.692050	1.294694	0.811813
H	-5.219106	2.167079	0.356123
H	-5.096392	0.892352	-1.845741
H	-6.573322	0.001164	-1.434121
H	-5.096792	-0.890548	-1.846068
H	-1.856124	-2.948457	-2.845036
H	-0.529316	-4.004679	-3.360164

H	-0.303375	-2.247272	-3.377451
H	1.783031	-2.534546	-1.950220
H	1.546111	-4.283340	-1.825575
H	1.674060	-3.297761	-0.352311
H	-2.014743	-4.157674	-0.619377
H	-0.565769	-4.321845	0.418507
H	-0.696778	-5.240005	-1.088801
H	4.125811	0.890316	-2.643329
H	4.127323	-0.889780	-2.644008
H	5.598211	0.001715	-3.094744
H	-2.014263	4.157874	-0.618390
H	-0.696126	5.240445	-1.086837
H	-0.565781	4.321795	0.420217
H	3.991420	2.155968	2.237631
H	1.617747	2.163341	2.924369
H	1.617314	-2.165897	2.922364
H	3.991005	-2.158376	2.235596
H	5.191578	-0.001132	1.917882

Intj_PhCN

C	4.833926	-0.001298	2.148802
C	5.292725	-0.000253	0.683877
C	6.116907	1.268953	0.401706
O	4.066161	-0.000161	-0.071739
C	4.121558	0.000576	-1.586436
C	6.117752	-1.268568	0.400171
K	1.327644	-0.001145	0.337213
O	-0.604794	-1.847979	0.802772
C	-0.286232	-3.041507	1.435161
C	-0.746132	-4.262097	0.590374
C	1.243902	-3.167373	1.657165
C	-0.982552	-3.133877	2.820881
K	-2.146367	-1.864833	-1.320694
K	-2.126493	-0.000011	1.877377
O	-3.636924	0.000893	-0.272557
C	-5.023919	0.001103	-0.281507
C	-5.571978	-1.253936	-1.012314
C	-5.571623	1.258274	-1.008915
C	-5.581650	-0.000748	1.166671
O	-0.603630	1.847082	0.803374
C	-0.284426	3.040176	1.436282
C	-0.981465	3.132704	2.821637
C	-0.742869	4.261373	0.591590
C	1.245672	3.164739	1.659188
K	-2.144811	1.865749	-1.320201
H	1.599880	-2.346958	2.296870
H	1.771784	-3.107783	0.696628
H	1.530894	-4.109616	2.142909
H	-0.652326	-2.303394	3.461667
H	-0.764743	-4.068540	3.354705
H	-2.073371	-3.066256	2.699631
H	-5.211121	1.277329	-2.047067
H	-5.220482	2.167522	-0.500025
H	-6.668469	1.298284	-1.037912
H	5.512591	-2.162401	0.586055
H	7.001611	-1.307793	1.047992
H	6.468620	-1.303467	-0.636779
H	6.467632	1.305368	-0.635246
H	7.000818	1.307944	1.049470
H	5.511190	2.162164	0.588765
H	-5.211061	-1.270496	-2.050359
H	-6.668831	-1.293340	-1.041826
H	-5.221534	-2.164692	-0.505618

H	-5.227272	-0.892853	1.702324
H	-6.678907	-0.000786	1.208954
H	-5.227284	0.890000	1.704598
H	-2.072270	3.065943	2.699769
H	-0.763241	4.067053	3.355844
H	-0.652219	2.301801	3.462385
H	1.600649	2.343743	2.298703
H	1.533124	4.106534	2.145527
H	1.774041	3.105181	0.698921
H	-1.835381	4.242850	0.459274
H	-0.267007	4.231010	-0.398591
H	-0.489196	5.225203	1.052074
H	4.230828	-0.892191	2.359285
H	4.229746	0.888652	2.360237
H	5.692533	-0.001137	2.830386
H	-1.838683	-4.242563	0.458539
H	-0.493105	-5.226264	1.050510
H	-0.270686	-4.231923	-0.400016
C	3.443324	-1.238111	-2.075749
C	2.167292	-1.227882	-2.548292
C	1.439720	0.000429	-2.740572
C	2.166654	1.228940	-2.547117
C	3.442678	1.239382	-2.074555
H	3.979704	-2.179083	-1.980516
H	1.683821	-2.166328	-2.816523
C	0.081074	0.000244	-3.037419
H	1.682699	2.167397	-2.814444
H	3.978579	2.180531	-1.978381
H	5.187868	0.000996	-1.832153
N	-1.089922	0.000114	-3.213621

TSk

C	-2.715529	-0.357599	-2.408861
Si	-4.277868	-0.532883	-1.374513
C	-5.114609	1.152332	-1.209360
C	-5.459068	-1.740608	-2.227298
O	-3.725694	-1.109261	0.119291
C	-4.442215	-1.675180	1.244744
C	-4.748272	-3.152791	0.958466
C	-3.495507	-1.561931	2.445984
C	-5.733508	-0.895616	1.532458
K	2.237574	1.361125	0.643681
O	1.313027	-0.629289	2.166523
C	1.390502	-0.747472	3.546169
C	2.203692	0.422881	4.163181
C	-0.023018	-0.749380	4.183714
C	2.093330	-2.072217	3.964580
K	-0.728359	-0.846617	0.414052
K	2.740427	-2.332016	0.774535
O	3.750835	-0.414821	-0.712274
C	5.094388	-0.205118	-0.975827
C	5.560797	1.171450	-0.429087
C	5.368453	-0.230840	-2.504465
C	5.965889	-1.305577	-0.311650
O	0.774055	-2.685578	-0.938598
C	0.365862	-3.951919	-1.325165
C	1.351882	-5.037178	-0.809520
C	0.300263	-4.065506	-2.873291
C	-1.040161	-4.279300	-0.757649
K	1.933355	-0.954093	-2.500270

H	-0.597985	-1.607171	3.810100
H	-0.558538	0.166353	3.904846
H	-0.000743	-0.811161	5.280418
H	1.565611	-2.933234	3.530015
H	2.121935	-2.215896	5.052838
H	3.136464	-2.082242	3.613240
H	4.770402	0.545003	-3.002687
H	5.084692	-1.209278	-2.919184
H	6.422266	-0.057169	-2.760406
H	-5.517409	0.162053	1.715354
H	-6.229101	-1.302320	2.420982
H	-6.441072	-0.967359	0.699483
H	-5.443603	-3.260492	0.120920
H	-5.199667	-3.629567	1.836431
H	-3.826734	-3.689606	0.710484
H	4.976355	1.977064	-0.895187
H	6.622735	1.375848	-0.621039
H	5.406148	1.213810	0.658518
H	5.815048	-1.294701	0.777024
H	7.040764	-1.181259	-0.500177
H	5.672308	-2.294375	-0.691992
H	2.364811	-4.832790	-1.184933
H	1.079190	-6.053831	-1.122932
H	1.379752	-5.029317	0.289860
H	-1.019585	-4.212739	0.338845
H	-1.392090	-5.284337	-1.028571
H	-1.774874	-3.553395	-1.129053
H	1.299881	-3.911026	-3.306704
H	-0.371837	-3.294669	-3.273648
H	-0.059473	-5.042867	-3.222115
H	-3.198650	-0.520035	2.608752
H	-2.594477	-2.166468	2.290828
H	-3.978010	-1.925459	3.359893
H	3.213201	0.443314	3.728470
H	2.310610	0.344335	5.253725
H	1.714920	1.380116	3.943688
H	0.443248	1.048054	-1.241817
H	-5.002685	-2.729021	-2.355292
H	-6.404900	-1.872630	-1.689199
H	-5.706601	-1.360274	-3.226948
H	-2.972968	-0.019540	-3.421304
H	-2.016904	0.378555	-1.990146
H	-2.190156	-1.315917	-2.507383
H	-5.307832	1.567649	-2.207022
H	-6.072298	1.103672	-0.680287
H	-4.469006	1.861278	-0.678746
O	-0.425186	1.839711	-0.440641
N	0.023462	3.197497	-0.213621
C	-0.694256	3.708298	1.007894
C	-0.344905	5.201166	1.215841
C	-2.229480	3.509478	0.977180
C	-0.146652	2.946178	2.228021
C	-0.570357	6.064086	-0.023080
H	-0.924854	5.574242	2.069992
H	0.715176	5.274013	1.498740
C	0.230078	5.474961	-1.182656
H	-1.637416	6.115333	-0.273055
H	-0.251354	7.095831	0.172790
C	-0.112822	3.997652	-1.484023
H	0.079215	6.056505	-2.101051
H	1.300168	5.543334	-0.938825
C	-1.491657	3.881804	-2.172635
C	0.949541	3.480000	-2.472336

H	-2.649101	3.693132	1.973730
H	-2.730881	4.186526	0.282194
H	-2.463386	2.483654	0.682681
H	-0.652272	3.277990	3.142388
H	-0.283922	1.866730	2.135690
H	0.922866	3.153265	2.363913
H	0.728921	2.456990	-2.789956
H	0.981723	4.126533	-3.358322
H	1.944087	3.485648	-2.009118
H	-1.821557	2.841209	-2.149947
H	-2.259243	4.501528	-1.702442
H	-1.414591	4.200436	-3.219156

Intk

C	-2.819735	-1.529105	-2.260175
Si	-4.337888	-0.568784	-1.690597
C	-4.713900	0.800657	-2.933836
C	-5.805854	-1.754412	-1.577393
O	-3.885399	0.075787	-0.187729
C	-4.693056	0.618303	0.889358
C	-5.336255	-0.533226	1.675562
C	-3.724062	1.384956	1.798733
C	-5.759119	1.581571	0.347712
K	2.377180	1.513925	-1.959052
O	1.067404	2.013162	0.303792
C	0.994087	3.317683	0.773263
C	-0.480433	3.747492	0.987798
C	1.736488	3.459757	2.130842
C	1.640936	4.313515	-0.227171
K	-0.943511	0.320614	0.054476
K	2.481945	0.158532	1.533097
O	3.721730	-0.375333	-0.702354
C	5.099568	-0.514370	-0.803216
C	5.700857	0.579626	-1.725099
C	5.475171	-1.899850	-1.392723
C	5.771044	-0.387985	0.591568
K	2.001026	-2.258076	-1.266357
O	0.621031	-1.619977	0.911053
C	0.210610	-2.595934	1.809172
C	1.114427	-2.602180	3.072816
C	0.275848	-4.008450	1.168828
C	-1.250125	-2.347610	2.271428
H	2.798051	3.200051	2.009295
H	1.293947	2.780118	2.873343
H	1.691434	4.476737	2.543142
H	2.703045	4.067974	-0.373612
H	1.590794	5.356382	0.113050
H	1.131409	4.255890	-1.199036
H	5.022309	-2.018775	-2.386382
H	5.097453	-2.700822	-0.740205
H	6.558753	-2.044219	-1.498654
H	-5.296185	2.387934	-0.230899
H	-6.317721	2.032341	1.175532
H	-6.481209	1.065240	-0.293737
H	-6.067587	-1.074633	1.069373
H	-5.852835	-0.149021	2.562628
H	-4.568123	-1.241279	2.003913
H	5.268706	0.501135	-2.732224
H	6.792256	0.507898	-1.824131
H	5.468834	1.576525	-1.322727
H	5.557580	0.600037	1.024704
H	6.862490	-0.504171	0.556076
H	5.376173	-1.158707	1.269044

H	2.161418	-2.770655	2.784247
H	0.838279	-3.380473	3.796636
H	1.047365	-1.633793	3.590293
H	-1.325087	-1.361837	2.752892
H	-1.607528	-3.096525	2.991017
H	-1.928838	-2.362108	1.407916
H	1.312565	-4.254379	0.894720
H	-0.337022	-4.035242	0.257872
H	-0.079171	-4.802177	1.839597
H	-3.220150	2.184938	1.245442
H	-2.971087	0.707808	2.220402
H	-4.259025	1.842407	2.638062
H	-1.036143	3.648426	0.045226
H	-0.582699	4.785225	1.332791
H	-0.952555	3.099473	1.739094
H	-5.608296	-2.580040	-0.884260
H	-6.735803	-1.265342	-1.265992
H	-5.987289	-2.193277	-2.567111
H	-3.054118	-2.099230	-3.168398
H	-1.971307	-0.880541	-2.520249
H	-2.480098	-2.247878	-1.503771
H	-4.824947	0.371469	-3.937914
H	-5.636212	1.344627	-2.703019
H	-3.894678	1.528822	-2.979624

7

O	0.349086	1.537497	-0.366489
N	0.660013	2.879399	0.038732
C	-0.402735	3.407342	0.962712
C	-0.092117	4.877158	1.333956
C	-1.844169	3.280260	0.418277
C	-0.321293	2.605088	2.276936
C	0.140983	5.777394	0.124517
H	-0.910912	5.258390	1.958306
H	0.813631	4.895240	1.957338
C	1.260730	5.177789	-0.721137
H	-0.778324	5.882639	-0.465275
H	0.412148	6.789597	0.451367
C	0.988244	3.720506	-1.163676
H	1.444154	5.784287	-1.617754
H	2.189710	5.195324	-0.132621
C	-0.073908	3.683806	-2.288200
C	2.311165	3.197958	-1.760420
H	-2.572935	3.415341	1.227380
H	-2.070911	4.020354	-0.353290
H	-1.978781	2.286606	-0.013431
H	-1.050115	2.986817	3.001997
H	-0.516317	1.541496	2.129844
H	0.672354	2.706109	2.732132
H	2.187596	2.245707	-2.280638
H	2.702122	3.915381	-2.492231
H	3.069659	3.066724	-0.980280
H	-0.428892	2.657314	-2.409550
H	-0.937330	4.322214	-2.084437
H	0.362274	4.021587	-3.237002
C	-2.430892	0.060477	-2.285856
Si	-4.132457	-0.030143	-1.483901
C	-4.979548	1.651005	-1.644546
C	-5.166762	-1.348188	-2.361007
O	-3.810430	-0.431703	0.129810
C	-4.692151	-0.837912	1.205998
C	-4.921853	-2.353403	1.112438
C	-3.959459	-0.491427	2.509062

C	-6.026433	-0.079755	1.154592
K	2.432899	0.979026	1.181569
O	1.174771	-1.104537	2.280267
C	1.184579	-1.408381	3.630944
C	2.005129	-0.359700	4.430723
C	-0.257505	-1.432044	4.202912
C	1.820800	-2.804032	3.885812
K	-0.882234	-0.718747	0.614499
K	2.315193	-2.670435	0.525541
O	3.503297	-0.649416	-0.627915
C	4.816805	-0.644518	-1.065424
C	5.637816	0.454098	-0.337731
C	4.891207	-0.370388	-2.592430
C	5.497044	-2.013737	-0.790884
O	0.227305	-2.401007	-1.120434
C	-0.151706	-3.551043	-1.796269
C	0.793375	-4.742024	-1.466286
C	-0.104512	-3.332080	-3.333461
C	-1.590778	-3.976703	-1.404378
K	1.364442	-0.249262	-2.097435
H	-0.851904	-2.191178	3.675140
H	-0.734064	-0.454770	4.050366
H	-0.295393	-1.662940	5.276367
H	1.258427	-3.576686	3.342138
H	1.832942	-3.086810	4.946968
H	2.862273	-2.814635	3.531729
H	4.440377	0.605670	-2.819252
H	4.334064	-1.145583	-3.137647
H	5.918112	-0.361573	-2.982030
H	-5.860557	1.001561	1.194187
H	-6.652331	-0.361156	2.008668
H	-6.589218	-0.312658	0.244329
H	-5.464158	-2.616668	0.199166
H	-5.504220	-2.711110	1.969591
H	-3.963471	-2.883812	1.102662
H	5.190212	1.439623	-0.525936
H	6.687266	0.495966	-0.659259
H	5.627083	0.270558	0.745972
H	5.482200	-2.228516	0.287279
H	6.543266	-2.052164	-1.123027
H	4.952212	-2.813765	-1.312140
H	1.828957	-4.495483	-1.742261
H	0.522535	-5.662056	-2.000584
H	0.756835	-4.968792	-0.390465
H	-1.642411	-4.147514	-0.320716
H	-1.920482	-4.894723	-1.910001
H	-2.301235	-3.179199	-1.653523
H	0.917965	-3.070793	-3.642293
H	-0.770412	-2.506764	-3.617393
H	-0.406973	-4.219394	-3.905892
H	-3.713105	0.575338	2.538729
H	-3.032652	-1.067479	2.609002
H	-4.582131	-0.726420	3.379390
H	3.040039	-0.335653	4.060022
H	2.042138	-0.568719	5.508505
H	1.566335	0.638398	4.298352
H	-4.695071	-2.335606	-2.298298
H	-6.184303	-1.433981	-1.962880
H	-5.256509	-1.093013	-3.425001
H	-2.535793	0.336702	-3.343430
H	-1.786514	0.809936	-1.806919
H	-1.913357	-0.905473	-2.242864
H	-4.999549	1.950572	-2.700552

H	-6.013567	1.649972	-1.284091
H	-4.428953	2.422869	-1.094736

TEMPO

O	2.018305	-0.099681	0.000000
N	0.756913	0.148652	0.000000
C	0.071396	0.023285	1.331608
C	-1.360502	0.590267	1.247139
C	0.071396	-1.459466	1.761399
C	0.892111	0.842909	2.341017
C	-2.124485	0.141683	0.000000
H	-1.895184	0.304319	2.161376
H	-1.305747	1.687608	1.246140
C	-1.360502	0.590267	-1.247139
H	-2.266641	-0.946402	0.000000
H	-3.128778	0.582595	0.000000
C	0.071396	0.023285	-1.331608
H	-1.895184	0.304319	-2.161376
H	-1.305747	1.687608	-1.246140
C	0.071396	-1.459466	-1.761399
C	0.892111	0.842909	-2.341017
H	-0.264305	-1.549181	2.800842
H	-0.589648	-2.072620	1.141246
H	1.085797	-1.861225	1.686490
H	0.409115	0.805413	3.323883
H	1.906270	0.448831	2.426670
H	0.956046	1.890184	2.026862
H	1.906270	0.448831	-2.426670
H	0.409115	0.805413	-3.323883
H	0.956046	1.890184	-2.026862
H	1.085797	-1.861225	-1.686490
H	-0.589648	-2.072620	-1.141246
H	-0.264305	-1.549181	-2.800842

TEMPO-H

C	-0.048612	0.032630	1.294820
N	-0.661778	0.447098	0.000000
C	-0.048612	0.032630	-1.294820
C	1.434534	0.465757	-1.251690
C	2.170083	-0.020315	0.000000
C	1.434534	0.465757	1.251690
O	-2.038240	-0.008294	0.000000
C	-0.187543	-1.469187	-1.634730
C	-0.764939	0.842336	-2.393580
C	-0.187543	-1.469187	1.634730
C	-0.764939	0.842336	2.393580
H	1.928146	0.104003	-2.162490
H	1.476777	1.563024	-1.280340
H	2.248586	-1.114710	0.000000
H	3.199462	0.359693	0.000000
H	1.928146	0.104003	2.162490
H	1.476777	1.563024	1.280340
H	0.056505	-1.632304	-2.691080
H	0.476903	-2.104649	-1.044710
H	-1.216495	-1.798568	-1.468480
H	-0.264950	0.700416	-3.358570
H	-1.805484	0.522147	-2.501600
H	-0.751073	1.910356	-2.150060
H	-1.805484	0.522147	2.501600
H	-0.264950	0.700416	3.358570
H	-0.751073	1.910356	2.150060
H	-1.216495	-1.798568	1.468480
H	0.476903	-2.104649	1.044710

H	0.056505	-1.632304	2.691080
H	-2.532100	0.826297	0.000000

O_2

O	0.000000	0.000000	0.607331
O	0.000000	0.000000	-0.607331

Intm

C	-4.348074	-0.767978	-2.843685
Si	-4.201261	0.639628	-1.596915
O	-3.787942	0.049356	-0.061602
C	-4.604529	-0.542188	0.978969
C	-5.351378	0.568672	1.732308
C	-2.763433	1.759335	-2.071335
C	-5.793366	1.662624	-1.591118
C	-5.585553	-1.570497	0.396670
C	-3.630539	-1.246039	1.932885
K	-0.833817	-0.249876	0.253418
O	0.659956	1.867599	0.984880
C	0.228986	2.901395	1.799920
C	1.166426	3.067215	3.027768
C	0.213474	4.247752	1.025411
C	-1.205875	2.631395	2.326155
K	1.713691	2.139530	-1.382316
O	3.616246	0.445752	-0.811028
C	4.953338	0.594736	-1.138655
C	5.828358	0.693779	0.140271
C	5.178358	1.883154	-1.976702
C	5.457591	-0.613449	-1.973740
K	2.636141	0.250719	1.631374
O	1.216655	-1.820999	0.938366
C	1.209591	-3.009670	1.651326
C	-0.237747	-3.423772	2.023711
C	2.021941	-2.868547	2.968252
C	1.839589	-4.161444	0.821125
K	2.159937	-1.676021	-1.519361
O	-0.226815	-2.951499	-2.433895
O	-0.876342	-1.882263	-2.369990
H	-1.220910	1.688851	2.891118
H	-1.904794	2.537080	1.484249
H	-1.580238	3.424866	2.987415
H	1.166934	2.145495	3.627600
H	0.870706	3.891261	3.690884
H	2.194247	3.262671	2.690101
H	4.869246	-0.699219	-2.898308
H	5.338444	-1.541953	-1.397416
H	6.515133	-0.533115	-2.258519
H	-4.641678	1.317862	2.099095
H	-5.890301	0.154359	2.592305
H	-6.079594	1.069416	1.088372
H	-6.311934	-1.099811	-0.274489
H	-6.147802	-2.056445	1.202027
H	-5.048947	-2.344872	-0.161389
H	4.582202	1.836986	-2.898998
H	6.226946	2.036451	-2.264996
H	4.861354	2.764620	-1.400628
H	5.509517	1.554175	0.745584
H	6.898593	0.814960	-0.074449
H	5.710133	-0.217180	0.743902
H	3.068680	-2.618237	2.740577
H	2.027552	-3.784165	3.574805
H	1.596433	-2.062979	3.583549

H	-0.701283	-2.642080	2.640758
H	-0.286846	-4.367558	2.583929
H	-0.835759	-3.542997	1.110370
H	2.877004	-3.908571	0.556942
H	1.268262	-4.310957	-0.105020
H	1.860176	-5.119062	1.358489
H	-2.926940	-0.525786	2.367639
H	-3.067873	-2.028140	1.411027
H	-4.169848	-1.719241	2.760660
H	1.228499	4.493281	0.679573
H	-0.141332	5.093095	1.630144
H	-0.441675	4.163847	0.147519
H	0.314101	0.091102	-2.206418
H	-6.685071	1.082548	-1.328050
H	-5.727209	2.512858	-0.902566
H	-5.957976	2.067898	-2.598073
H	-4.476756	-0.360467	-3.854946
H	-3.436530	-1.376851	-2.848368
H	-5.199451	-1.427720	-2.642791
H	-2.994450	2.285291	-3.007128
H	-2.578702	2.518722	-1.301059
H	-1.832701	1.199828	-2.238481

TSn

C	-3.649141	-1.994079	-2.019416
Si	-4.494038	-0.409708	-1.455086
O	-3.906067	-0.125342	0.112300
C	-4.532718	0.412643	1.302352
C	-5.139835	1.793500	1.012714
C	-3.992506	1.037202	-2.557153
C	-6.367161	-0.657358	-1.558028
C	-5.596442	-0.565518	1.823561
C	-3.415803	0.544962	2.347230
K	-0.949720	-0.035288	-0.014709
O	0.808765	1.949620	0.433576
C	0.443756	3.190023	0.940081
C	0.345769	3.144695	2.489516
C	1.484495	4.282445	0.565813
C	-0.930006	3.639573	0.376785
K	2.504887	1.931097	-1.620650
O	3.838884	0.005712	-0.439126
C	5.223615	-0.075468	-0.447463
C	5.784866	-0.032617	0.999440
C	5.843393	1.104715	-1.242208
C	5.699206	-1.397913	-1.107917
K	2.355124	0.228974	1.704245
O	0.856560	-1.754369	0.888384
C	0.609860	-2.898860	1.632038
C	-0.911690	-3.096875	1.857163
C	1.295699	-2.812552	3.023289
C	1.155121	-4.163257	0.912201
K	2.298056	-1.921317	-1.328685
O	-0.175363	-1.232707	-2.436041
O	-0.255632	-0.063671	-3.059964
H	-1.717366	2.936080	0.680522
H	-0.895873	3.649402	-0.719855
H	-1.230241	4.638530	0.721182
H	-0.355177	2.357206	2.797002
H	0.007575	4.092300	2.929886
H	1.328414	2.913188	2.926986
H	5.333344	-1.451408	-2.142710
H	5.304413	-2.260027	-0.550555

H	6.792436	-1.497205	-1.136390
H	-4.376838	2.474224	0.620002
H	-5.550108	2.232670	1.929230
H	-5.953512	1.729121	0.282824
H	-6.435417	-0.657557	1.129315
H	-5.994431	-0.219934	2.784464
H	-5.157382	-1.558125	1.971181
H	5.476066	1.091416	-2.277623
H	6.940557	1.073602	-1.276324
H	5.553409	2.060393	-0.781640
H	5.491213	0.908170	1.486937
H	6.880201	-0.100344	1.041766
H	5.375769	-0.869032	1.583875
H	2.382301	-2.698087	2.900696
H	1.124125	-3.700772	3.645888
H	0.914002	-1.941584	3.575026
H	-1.321132	-2.235154	2.402119
H	-1.148757	-4.000113	2.435476
H	-1.428217	-3.168730	0.890934
H	2.243408	-4.080202	0.773972
H	0.681250	-4.268472	-0.073889
H	0.967629	-5.090201	1.469894
H	-2.658178	1.268779	2.025976
H	-2.936049	-0.424955	2.520539
H	-3.819844	0.897994	3.302279
H	2.486943	3.977120	0.897280
H	1.263549	5.257737	1.019217
H	1.508840	4.434529	-0.523498
H	0.825649	0.271115	-3.379355
H	-6.699536	-1.543201	-1.005707
H	-6.948688	0.202172	-1.207374
H	-6.630657	-0.814793	-2.612274
H	-4.020384	-2.284926	-3.010753
H	-2.561438	-1.887324	-2.104972
H	-3.861368	-2.819895	-1.329392
H	-4.380847	0.897450	-3.574252
H	-4.379886	1.991642	-2.181541
H	-2.901871	1.121747	-2.641992

Intn

C	3.209535	1.382461	-2.296008
Si	4.525632	0.320116	-1.464884
C	4.731001	-1.304580	-2.402040
C	6.156929	1.275496	-1.471597
O	3.912749	0.029762	0.090038
C	4.581251	-0.333895	1.325398
C	5.287279	0.899937	1.906378
C	3.477316	-0.793882	2.286999
C	5.574070	-1.481836	1.093364
K	0.992205	-0.079574	0.020270
O	-0.716030	1.790737	0.754493
C	-0.397387	2.943462	1.457876
C	-0.926652	2.865318	2.916196
C	-1.024593	4.198418	0.791399
C	1.138631	3.153633	1.514686
K	-2.276018	-0.103449	1.744802
O	-3.836343	0.112921	-0.324527
C	-5.222112	0.174612	-0.259205
C	-5.864959	-1.012902	-1.022486
C	-5.748343	1.491237	-0.889510
C	-5.703459	0.120268	1.215793
K	-2.326470	1.962060	-1.363110

K	-2.519756	-1.762478	-1.589020
O	-0.845432	-1.941986	0.492950
C	-0.567993	-3.206200	0.996993
C	-1.715028	-4.203576	0.676219
C	0.739085	-3.774387	0.383733
C	-0.402123	-3.157326	2.540174
O	-0.326194	0.101616	-2.352339
O	-0.248120	0.011928	-3.673476
H	1.594998	-3.137311	0.647556
H	0.659651	-3.790821	-0.710860
H	0.967952	-4.792400	0.726580
H	0.378133	-2.433234	2.810356
H	-0.131313	-4.127870	2.976978
H	-1.341501	-2.835609	3.013526
H	-5.443589	1.549193	-1.943388
H	-5.330017	2.357051	-0.355531
H	-6.842507	1.577727	-0.853682
H	5.067132	-2.353418	0.665975
H	6.033186	-1.784751	2.041036
H	6.381527	-1.182979	0.416615
H	6.106757	1.233155	1.263898
H	5.705215	0.673065	2.893846
H	4.576402	1.725924	2.015749
H	-5.556638	-0.989849	-2.076601
H	-6.962695	-0.998756	-0.994710
H	-5.534309	-1.965268	-0.582895
H	-5.369908	-0.816775	1.684987
H	-6.795915	0.169998	1.315993
H	-5.278980	0.963363	1.779966
H	-2.021281	2.761007	2.915579
H	-0.680851	3.752885	3.514150
H	-0.494385	1.991269	3.424142
H	1.615917	2.306685	2.027486
H	1.429751	4.069496	2.046552
H	1.545200	3.209693	0.496297
H	-2.119743	4.102896	0.761366
H	-0.652068	4.304025	-0.237498
H	-0.792096	5.130113	1.323518
H	2.941066	-1.658926	1.881019
H	2.763310	0.017082	2.475483
H	3.902882	-1.088169	3.252431
H	-2.670654	-3.808811	1.047494
H	-1.560912	-5.193370	1.125609
H	-1.802625	-4.355233	-0.409886
H	-1.264801	-0.010993	-4.027459
H	6.061315	2.244409	-0.968611
H	6.987288	0.731904	-1.007356
H	6.444023	1.474020	-2.512476
H	3.577211	1.739188	-3.266540
H	2.274187	0.847273	-2.498076
H	2.973936	2.267193	-1.691409
H	4.984247	-1.106815	-3.451402
H	5.524919	-1.932030	-1.982046
H	3.802730	-1.888833	-2.394567

TSo

C	-3.502464	-1.948093	-2.147725
Si	-4.384033	-0.383525	-1.580741
C	-6.246277	-0.627219	-1.802257
O	-3.892139	-0.162810	0.027794
C	-4.580565	0.348576	1.195432
C	-3.518590	0.461899	2.297925

C	-3.816681	1.099155	-2.599760
C	-5.178508	1.733014	0.905390
C	-5.664366	-0.645556	1.639448
K	-0.933537	-0.084682	0.068761
O	0.915553	-1.805570	0.948619
C	0.648682	-2.929953	1.715621
C	1.173162	-4.218325	1.023117
C	-0.876257	-3.097887	1.942825
C	1.335206	-2.824357	3.104752
K	2.389545	0.222952	1.714256
O	3.727296	0.033689	-0.534475
C	5.113030	0.053270	-0.619108
C	5.646035	-1.232576	-1.307595
C	5.748376	0.137390	0.795234
C	5.603037	1.273567	-1.441995
K	2.334711	-2.041766	-1.255559
K	2.216784	1.910715	-1.621417
O	0.735558	1.927651	0.583181
C	0.393062	3.150890	1.144909
C	-0.952889	3.667878	0.572751
C	0.252621	3.029688	2.686810
C	1.476314	4.225901	0.852835
O	-0.032420	-1.152260	-2.335207
O	0.242234	0.136182	-2.882527
H	-1.763546	2.966153	0.812233
H	-0.889552	3.742082	-0.520271
H	-1.238012	4.651974	0.968699
H	-0.479034	2.250083	2.936859
H	-0.068347	3.964484	3.165657
H	1.215362	2.745434	3.137324
H	5.227977	-1.315682	-2.320364
H	5.349523	-2.120574	-0.729116
H	6.740107	-1.251682	-1.397584
H	-4.399993	2.425389	0.567451
H	-5.637050	2.149748	1.809340
H	-5.953983	1.681822	0.134041
H	-6.465343	-0.728030	0.900292
H	-6.114347	-0.322261	2.585025
H	-5.227174	-1.638604	1.789780
H	5.185831	1.233954	-2.457446
H	6.696376	1.321598	-1.531622
H	5.269792	2.206330	-0.964132
H	5.421347	1.058204	1.299507
H	6.846247	0.143589	0.775698
H	5.430161	-0.723323	1.400984
H	2.423092	-2.727562	2.979255
H	1.150661	-3.696646	3.745819
H	0.966457	-1.936280	3.637351
H	-1.272015	-2.218194	2.469020
H	-1.128669	-3.984160	2.540372
H	-1.392949	-3.183348	0.977545
H	2.263169	-4.157221	0.886137
H	0.699488	-4.335944	0.038128
H	0.968635	-5.130370	1.598912
H	-2.747102	1.192408	2.029106
H	-3.046428	-0.510792	2.476949
H	-3.971399	0.795692	3.237873
H	2.458047	3.876399	1.201078
H	1.267763	5.187750	1.339723
H	1.544846	4.421438	-0.227516
H	0.984610	0.111373	-3.656116
H	-6.608856	-1.527182	-1.293359
H	-6.846015	0.223170	-1.460173

H	-6.450846	-0.754816	-2.873382
H	-3.782163	-2.188035	-3.181583
H	-2.410991	-1.846460	-2.127824
H	-3.777040	-2.804695	-1.520248
H	-4.098915	0.972020	-3.652820
H	-4.265862	2.034945	-2.246835
H	-2.726182	1.219355	-2.574906

OH radical

O	0.000000	0.000000	0.109212
H	0.000000	0.000000	-0.873700

Intp

C	-2.875603	-2.007275	-2.124397
Si	-3.951755	-0.494960	-1.821759
C	-3.246515	0.970620	-2.776285
C	-5.723130	-0.856898	-2.386884
O	-3.813783	-0.189833	-0.156229
C	-4.719611	0.394002	0.806479
C	-5.869125	-0.583267	1.095881
C	-3.898870	0.607968	2.086640
C	-5.252862	1.743727	0.302814
K	-0.945028	-0.034069	0.466489
O	0.941259	-1.791007	1.205148
C	0.750714	-2.837783	2.089780
C	1.668974	-2.685032	3.333703
C	1.078566	-4.199243	1.417135
C	-0.720919	-2.887770	2.582188
K	2.613858	0.192480	1.545200
O	3.476746	-0.056215	-0.925276
C	4.797619	-0.071359	-1.334994
C	5.083317	1.091162	-2.324844
C	5.140769	-1.406193	-2.051605
C	5.755125	0.082883	-0.121897
K	1.774923	-2.048272	-1.277616
K	1.670774	1.701192	-1.714357
O	0.827276	1.960283	0.779045
C	0.685697	3.202437	1.371085
C	0.968252	4.342309	0.352570
C	-0.753441	3.395797	1.916987
C	1.675356	3.370457	2.558057
O	0.014229	-0.265844	-1.987756
H	-0.976601	2.612325	2.653882
H	-1.476469	3.310570	1.094247
H	-0.906943	4.369378	2.402421
H	1.485754	2.595949	3.314860
H	1.595489	4.346669	3.055034
H	2.710152	3.263494	2.201615
H	4.492704	-1.533946	-2.930328
H	4.971076	-2.250430	-1.368152
H	6.182619	-1.460153	-2.395018
H	-4.424591	2.425617	0.082169
H	-5.888515	2.213542	1.062038
H	-5.852613	1.623813	-0.605430
H	-6.494859	-0.737905	0.213120
H	-6.509054	-0.198759	1.898498
H	-5.468746	-1.553098	1.410555
H	4.434920	0.995595	-3.207414
H	6.123420	1.118001	-2.676678
H	4.870467	2.054145	-1.839193
H	5.551753	1.031454	0.395018

H	6.817250	0.076193	-0.401875
H	5.591387	-0.740031	0.588324
H	2.722722	-2.668569	3.020363
H	1.551511	-3.497094	4.064037
H	1.445400	-1.739667	3.848480
H	-0.977122	-1.945086	3.086211
H	-0.913718	-3.706997	3.288323
H	-1.397040	-3.015818	1.725799
H	2.125258	-4.206994	1.080449
H	0.430092	-4.347394	0.542079
H	0.938058	-5.059532	2.085393
H	-3.096665	1.336589	1.923031
H	-3.461471	-0.338908	2.424688
H	-4.531336	0.994026	2.893649
H	1.997501	4.261521	-0.026919
H	0.853854	5.346437	0.782512
H	0.274658	4.262576	-0.496565
H	-6.136972	-1.748127	-1.901617
H	-6.419550	-0.026583	-2.225090
H	-5.704564	-1.054202	-3.466894
H	-3.011509	-2.372688	-3.150879
H	-1.816707	-1.736952	-2.006440
H	-3.122163	-2.827760	-1.439466
H	-3.371041	0.824520	-3.857309
H	-3.721802	1.922040	-2.510478
H	-2.169117	1.038074	-2.574973

References

1. Perry, R. H.; Cahill, T. J.; Roizen, J. L.; Du Bois, J.; Zare, R. N., Capturing fleeting intermediates in a catalytic C–H amination reaction cycle. *Proc. Natl. Acad. Sci. U.S.A* **2012,** *109* (45), 18295-18299.
2. Boeser, C. L.; Holder, J. C.; Taylor, B. L. H.; Houk, K. N.; Stoltz, B. M.; Zare, R. N., Mechanistic analysis of an asymmetric palladium-catalyzed conjugate addition of arylboronic acids to [small beta]-substituted cyclic enones. *Chemical Sci.* **2015,** *6* (3), 1917-1922.
3. Ingram, A. J.; Solis-Ibarra, D.; Zare, R. N.; Waymouth, R. M., Trinuclear Pd3O2 Intermediate in Aerobic Oxidation Catalysis. *Angew. Chem. Int. Ed.* **2014,** *53* (22), 5648-5652.
4. Perry, R. H.; Brownell, K. R.; Chingin, K.; Cahill, T. J.; Waymouth, R. M.; Zare, R. N., Transient Ru-methyl formate intermediates generated with bifunctional transfer hydrogenation catalysts. *Proc. Natl. Acad. Sci. U.S.A* **2012,** *109* (7), 2246-2250.
5. Perry, R. H.; Splendore, M.; Chien, A.; Davis, N. K.; Zare, R. N., Detecting Reaction Intermediates in Liquids on the Millisecond Time Scale Using Desorption Electrospray Ionization. *Angew. Chem. Int. Ed.* **2011,** *50* (1), 250-254.
6. Brownell, K. R.; McCrory, C. C. L.; Chidsey, C. E. D.; Perry, R. H.; Zare, R. N.; Waymouth, R. M., Electrooxidation of Alcohols Catalyzed by Amino Alcohol Ligated Ruthenium Complexes. *J. Am. Chem. Soc.* **2013,** *135* (38), 14299-14305.
7. Takáts, Z.; Wiseman, J. M.; Gologan, B.; Cooks, R. G., Mass Spectrometry Sampling Under Ambient Conditions with Desorption Electrospray Ionization. *Science* **2004,** *306* (5695), 471-473.
8. Toutov, A. A.; Liu, W.-B.; Betz, K. N.; Fedorov, A.; Stoltz, B. M.; Grubbs, R. H., Silylation of C-H bonds in aromatic heterocycles by an Earth-abundant metal catalyst. *Nature* **2015,** *518* (7537), 80-84.
9. Venter, A.; Sojka, P. E.; Cooks, R. G., Droplet Dynamics and Ionization Mechanisms in Desorption Electrospray Ionization Mass Spectrometry. *Anal. Chem.* **2006,** *78* (24), 8549-8555.